Pyro Documentation

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Pyro Core:

CHAPTER 1

Getting Started

- Install Pyro.
- Learn the basic concepts of Pyro: models and inference.
- Dive in to other tutorials and examples.

CHAPTER 2

Primitives

get_param_store()
Returns the ParamStore

clear_param_store()
Clears the ParamStore. This is especially useful if you're working in a REPL.

param(*name*, **args*, ***kwargs*)
Saves the variable as a parameter in the param store. To interact with the param store or write to disk, see Parameters.

Parameters

- **name** (*str*) – name of parameter
- **init_tensor** (*torch.Tensor or callable*) – initial tensor or lazy callable that returns a tensor. For large tensors, it may be cheaper to write e.g. `lambda: torch.randn(100000)`, which will only be evaluated on the initial statement.
- **constraint** (*torch.distributions.constraints.Constraint*) – torch constraint, defaults to `constraints.real`.
- **event_dim** (*int*) – (optional) number of rightmost dimensions unrelated to baching. Dimension to the left of this will be considered batch dimensions; if the param statement is inside a subsampled plate, then corresponding batch dimensions of the parameter will be correspondingly subsampled. If unspecified, all dimensions will be considered event dims and no subsampling will be performed.

Returns parameter

Return type torch.Tensor

sample(*name*, *fn*, **args*, ***kwargs*)
Calls the stochastic function *fn* with additional side-effects depending on *name* and the enclosing context (e.g. an inference algorithm). See Intro I and Intro II for a discussion.

Parameters

- **name** – name of sample

- **fn** – distribution class or function
- **obs** – observed datum (optional; should only be used in context of inference) optionally specified in kwargs
- **infer** (*dict*) – Optional dictionary of inference parameters specified in kwargs. See inference documentation for details.

Returns sample

factor(*name*, *log_factor*)

Factor statement to add arbitrary log probability factor to a probabilisitic model.

Parameters

- **name** (*str*) – Name of the trivial sample
- **log_factor** (*torch.Tensor*) – A possibly batched log probability factor.

deterministic(*name*, *value*, *event_dim=None*)

EXPERIMENTAL Deterministic statement to add a *Delta* site with name *name* and value *value* to the trace. This is useful when we want to record values which are completely determined by their parents. For example:

```
x = sample("x", dist.Normal(0, 1))
x2 = deterministic("x2", x ** 2)
```

Note: The site does not affect the model density. This currently converts to a *sample()* statement, but may change in the future.

Parameters

- **name** (*str*) – Name of the site.
- **value** (*torch.Tensor*) – Value of the site.
- **event_dim** (*int*) – Optional event dimension, defaults to *value.ndim*.

subsample(*data*, *event_dim*)

EXPERIMENTAL Subsampling statement to subsample data based on enclosing *plate* s.

This is typically called on arguments to `model()` when subsampling is performed automatically by *plate* s by passing either the `subsample` or `subsample_size` kwarg. For example the following are equivalent:

```
# Version 1. using indexing
def model(data):
    with pyro.plate("data", len(data), subsample_size=10, dim=-data.dim()) as ind:
        data = data[ind]
        # ...

# Version 2. using pyro.subsample()
def model(data):
    with pyro.plate("data", len(data), subsample_size=10, dim=-data.dim()):
        data = pyro.subsample(data, event_dim=0)
        # ...
```

Parameters

- **data** (*Tensor*) – A tensor of batched data.

- **event_dim** (*int*) – The event dimension of the data tensor. Dimensions to the left are considered batch dimensions.

Returns A subsampled version of `data`

Return type Tensor

class plate(*name*, *size=None*, *subsample_size=None*, *subsample=None*, *dim=None*, *use_cuda=None*, *device=None*)

Bases: *pyro.poutine.plate_messenger.PlateMessenger*

Construct for conditionally independent sequences of variables.

`plate` can be used either sequentially as a generator or in parallel as a context manager (formerly `irange` and `iarange`, respectively).

Sequential *plate* is similar to `range()` in that it generates a sequence of values.

Vectorized *plate* is similar to `torch.arange()` in that it yields an array of indices by which other tensors can be indexed. *plate* differs from `torch.arange()` in that it also informs inference algorithms that the variables being indexed are conditionally independent. To do this, *plate* is a provided as context manager rather than a function, and users must guarantee that all computation within an *plate* context is conditionally independent:

```
with plate("name", size) as ind:
    # ...do conditionally independent stuff with ind...
```

Additionally, *plate* can take advantage of the conditional independence assumptions by subsampling the indices and informing inference algorithms to scale various computed values. This is typically used to subsample minibatches of data:

```
with plate("data", len(data), subsample_size=100) as ind:
    batch = data[ind]
    assert len(batch) == 100
```

By default `subsample_size=False` and this simply yields a `torch.arange(0, size)`. If `0 < subsample_size <= size` this yields a single random batch of indices of size `subsample_size` and scales all log likelihood terms by `size/batch_size`, within this context.

Warning: This is only correct if all computation is conditionally independent within the context.

Parameters

- **name** (*str*) – A unique name to help inference algorithms match *plate* sites between models and guides.
- **size** (*int*) – Optional size of the collection being subsampled (like *stop* in builtin *range*).
- **subsample_size** (*int*) – Size of minibatches used in subsampling. Defaults to *size*.
- **subsample** (Anything supporting *len()*.) – Optional custom subsample for user-defined subsampling schemes. If specified, then *subsample_size* will be set to *len(subsample)*.
- **dim** (*int*) – An optional dimension to use for this independence index. If specified, `dim` should be negative, i.e. should index from the right. If not specified, `dim` is set to the rightmost dim that is left of all enclosing `plate` contexts.
- **use_cuda** (*bool*) – DEPRECATED, use the *device* arg instead. Optional bool specifying whether to use cuda tensors for *subsample* and *log_prob*. Defaults to `torch.Tensor.is_cuda`.

- **device** (*str*) – Optional keyword specifying which device to place the results of *subsample* and *log_prob* on. By default, results are placed on the same device as the default tensor.

Returns A reusabe context manager yielding a single 1-dimensional `torch.Tensor` of indices.

Examples:

```
>>> # This version declares sequential independence and subsamples data:
>>> for i in plate('data', 100, subsample_size=10):
...     if z[i]:  # Control flow in this example prevents vectorization.
...         obs = sample('obs_{}'.format(i), dist.Normal(loc, scale),␣
↪obs=data[i])
```

```
>>> # This version declares vectorized independence:
>>> with plate('data'):
...     obs = sample('obs', dist.Normal(loc, scale), obs=data)
```

```
>>> # This version subsamples data in vectorized way:
>>> with plate('data', 100, subsample_size=10) as ind:
...     obs = sample('obs', dist.Normal(loc, scale), obs=data[ind])
```

```
>>> # This wraps a user-defined subsampling method for use in pyro:
>>> ind = torch.randint(0, 100, (10,)).long() # custom subsample
>>> with plate('data', 100, subsample=ind):
...     obs = sample('obs', dist.Normal(loc, scale), obs=data[ind])
```

```
>>> # This reuses two different independence contexts.
>>> x_axis = plate('outer', 320, dim=-1)
>>> y_axis = plate('inner', 200, dim=-2)
>>> with x_axis:
...     x_noise = sample("x_noise", dist.Normal(loc, scale))
...     assert x_noise.shape == (320,)
>>> with y_axis:
...     y_noise = sample("y_noise", dist.Normal(loc, scale))
...     assert y_noise.shape == (200, 1)
>>> with x_axis, y_axis:
...     xy_noise = sample("xy_noise", dist.Normal(loc, scale))
...     assert xy_noise.shape == (200, 320)
```

See SVI Part II for an extended discussion.

class iarange(**args*, ***kwargs*)

Bases: *pyro.primitives.plate*

class irange(**args*, ***kwargs*)

Bases: *pyro.poutine.subsample_messenger.SubsampleMessenger*

plate_stack(*prefix*, *sizes*, *rightmost_dim=-1*)

Create a contiguous stack of *plate* s with dimensions:

```
rightmost_dim - len(sizes), ..., rightmost_dim
```

Parameters

- **prefix** (*str*) – Name prefix for plates.
- **sizes** (*iterable*) – An iterable of plate sizes.

- **rightmost_dim** (*int*) – The rightmost dim, counting from the right.

module(*name*, *nn_module*, *update_module_params=False*)
Takes a torch.nn.Module and registers its parameters with the ParamStore. In conjunction with the ParamStore save() and load() functionality, this allows the user to save and load modules.

Parameters

- **name** (*str*) – name of module
- **nn_module** (*torch.nn.Module*) – the module to be registered with Pyro
- **update_module_params** – determines whether Parameters in the PyTorch module get overridden with the values found in the ParamStore (if any). Defaults to *False*

Returns torch.nn.Module

random_module(*name*, *nn_module*, *prior*, **args*, ***kwargs*)

Warning: The *random_module* primitive is deprecated, and will be removed in a future release. Use *PyroModule* instead to to create Bayesian modules from `torch.nn.Module` instances. See the Bayesian Regression tutorial for an example.

Places a prior over the parameters of the module *nn_module*. Returns a distribution (callable) over *nn.Module*s, which upon calling returns a sampled *nn.Module*.

Parameters

- **name** (*str*) – name of pyro module
- **nn_module** (*torch.nn.Module*) – the module to be registered with pyro
- **prior** – pyro distribution, stochastic function, or python dict with parameter names as keys and respective distributions/stochastic functions as values.

Returns a callable which returns a sampled module

barrier(*data*)
EXPERIMENTAL Ensures all values in `data` are ground, rather than lazy funsor values. This is useful in combination with `pyro.poutine.collapse()`.

enable_validation(*is_validate=True*)
Enable or disable validation checks in Pyro. Validation checks provide useful warnings and errors, e.g. NaN checks, validating distribution arguments and support values, etc. which is useful for debugging. Since some of these checks may be expensive, we recommend turning this off for mature models.

Parameters **is_validate** (*bool*) – (optional; defaults to True) whether to enable validation checks.

validation_enabled(*is_validate=True*)
Context manager that is useful when temporarily enabling/disabling validation checks.

Parameters **is_validate** (*bool*) – (optional; defaults to True) temporary validation check override.

trace(*fn=None*, *ignore_warnings=False*, *jit_options=None*)
Lazy replacement for `torch.jit.trace()` that works with Pyro functions that call `pyro.param()`.

The actual compilation artifact is stored in the `compiled` attribute of the output. Call diagnostic methods on this attribute.

Example:

```
def model(x):
    scale = pyro.param("scale", torch.tensor(0.5), constraint=constraints.
↪positive)
    return pyro.sample("y", dist.Normal(x, scale))

@pyro.ops.jit.trace
def model_log_prob_fn(x, y):
    cond_model = pyro.condition(model, data={"y": y})
    tr = pyro.poutine.trace(cond_model).get_trace(x)
    return tr.log_prob_sum()
```

Parameters

- **fn** (*callable*) – The function to be traced.
- **ignore_warnins** (*bool*) – Whether to ignore jit warnings.
- **jit_options** (*dict*) – Optional dict of options to pass to `torch.jit.trace()`, e.g. `{"optimize": False}`.

CHAPTER 3

Inference

In the context of probabilistic modeling, learning is usually called inference. In the particular case of Bayesian inference, this often involves computing (approximate) posterior distributions. In the case of parameterized models, this usually involves some sort of optimization. Pyro supports multiple inference algorithms, with support for stochastic variational inference (SVI) being the most extensive. Look here for more inference algorithms in future versions of Pyro.

See Intro II for a discussion of inference in Pyro.

3.1 SVI

class SVI(*model*, *guide*, *optim*, *loss*, *loss_and_grads=None*, *num_samples=0*, *num_steps=0*, ***kwargs*)

Bases: *pyro.infer.abstract_infer.TracePosterior*

Parameters

- **model** – the model (callable containing Pyro primitives)
- **guide** – the guide (callable containing Pyro primitives)
- **optim** (PyroOptim) – a wrapper a for a PyTorch optimizer
- **loss** (pyro.infer.elbo.ELBO) – an instance of a subclass of *ELBO*. Pyro provides three built-in losses: *Trace_ELBO*, *TraceGraph_ELBO*, and *TraceEnum_ELBO*. See the *ELBO* docs to learn how to implement a custom loss.
- **num_samples** – (DEPRECATED) the number of samples for Monte Carlo posterior approximation
- **num_steps** – (DEPRECATED) the number of optimization steps to take in `run()`

A unified interface for stochastic variational inference in Pyro. The most commonly used loss is `loss=Trace_ELBO()`. See the tutorial SVI Part I for a discussion.

evaluate_loss(**args*, ***kwargs*)

Returns estimate of the loss

Return type float

Evaluate the loss function. Any args or kwargs are passed to the model and guide.

run(**args*, ***kwargs*)

> **Warning:** This method is deprecated, and will be removed in a future release. For inference, use *step()* directly, and for predictions, use the *Predictive* class.

step(**args*, ***kwargs*)

Returns estimate of the loss

Return type float

Take a gradient step on the loss function (and any auxiliary loss functions generated under the hood by *loss_and_grads*). Any args or kwargs are passed to the model and guide

3.2 ELBO

class ELBO(*num_particles=1*, *max_plate_nesting=inf*, *max_iarange_nesting=None*, *vectorize_particles=False*, *strict_enumeration_warning=True*, *ignore_jit_warnings=False*, *jit_options=None*, *retain_graph=None*, *tail_adaptive_beta=-1.0*)

Bases: object

ELBO is the top-level interface for stochastic variational inference via optimization of the evidence lower bound.

Most users will not interact with this base class *ELBO* directly; instead they will create instances of derived classes: *Trace_ELBO*, *TraceGraph_ELBO*, or *TraceEnum_ELBO*.

Parameters

- **num_particles** – The number of particles/samples used to form the ELBO (gradient) estimators.
- **max_plate_nesting** (*int*) – Optional bound on max number of nested `pyro.plate()` contexts. This is only required when enumerating over sample sites in parallel, e.g. if a site sets `infer={"enumerate": "parallel"}`. If omitted, ELBO may guess a valid value by running the (model,guide) pair once, however this guess may be incorrect if model or guide structure is dynamic.
- **vectorize_particles** (*bool*) – Whether to vectorize the ELBO computation over *num_particles*. Defaults to False. This requires static structure in model and guide.
- **strict_enumeration_warning** (*bool*) – Whether to warn about possible misuse of enumeration, i.e. that *pyro.infer.traceenum_elbo.TraceEnum_ELBO* is used iff there are enumerated sample sites.
- **ignore_jit_warnings** (*bool*) – Flag to ignore warnings from the JIT tracer. When this is True, all `torch.jit.TracerWarning` will be ignored. Defaults to False.
- **jit_options** (*bool*) – Optional dict of options to pass to `torch.jit.trace()` , e.g. `{"check_trace": True}`.
- **retain_graph** (*bool*) – Whether to retain autograd graph during an SVI step. Defaults to None (False).

- **tail_adaptive_beta** (*float*) – Exponent beta with `-1.0 <= beta < 0.0` for use with *TraceTailAdaptive_ELBO*.

References

[1] *Automated Variational Inference in Probabilistic Programming* David Wingate, Theo Weber

[2] *Black Box Variational Inference*, Rajesh Ranganath, Sean Gerrish, David M. Blei

class Trace_ELBO(*num_particles=1*, *max_plate_nesting=inf*, *max_iarange_nesting=None*, *vectorize_particles=False*, *strict_enumeration_warning=True*, *ignore_jit_warnings=False*, *jit_options=None*, *retain_graph=None*, *tail_adaptive_beta=-1.0*)

Bases: *pyro.infer.elbo.ELBO*

A trace implementation of ELBO-based SVI. The estimator is constructed along the lines of references [1] and [2]. There are no restrictions on the dependency structure of the model or the guide. The gradient estimator includes partial Rao-Blackwellization for reducing the variance of the estimator when non-reparameterizable random variables are present. The Rao-Blackwellization is partial in that it only uses conditional independence information that is marked by `plate` contexts. For more fine-grained Rao-Blackwellization, see *TraceGraph_ELBO*.

References

[1] Automated Variational Inference in Probabilistic Programming, David Wingate, Theo Weber

[2] Black Box Variational Inference, Rajesh Ranganath, Sean Gerrish, David M. Blei

loss(*model*, *guide*, **args*, ***kwargs*)

Returns returns an estimate of the ELBO

Return type float

Evaluates the ELBO with an estimator that uses num_particles many samples/particles.

differentiable_loss(*model*, *guide*, **args*, ***kwargs*)

Computes the surrogate loss that can be differentiated with autograd to produce gradient estimates for the model and guide parameters

loss_and_grads(*model*, *guide*, **args*, ***kwargs*)

Returns returns an estimate of the ELBO

Return type float

Computes the ELBO as well as the surrogate ELBO that is used to form the gradient estimator. Performs backward on the latter. Num_particle many samples are used to form the estimators.

class JitTrace_ELBO(*num_particles=1*, *max_plate_nesting=inf*, *max_iarange_nesting=None*, *vectorize_particles=False*, *strict_enumeration_warning=True*, *ignore_jit_warnings=False*, *jit_options=None*, *retain_graph=None*, *tail_adaptive_beta=-1.0*)

Bases: *pyro.infer.trace_elbo.Trace_ELBO*

Like *Trace_ELBO* but uses `pyro.ops.jit.compile()` to compile *loss_and_grads()*.

This works only for a limited set of models:

- Models must have static structure.
- Models must not depend on any global data (except the param store).
- All model inputs that are tensors must be passed in via `*args`.
- All model inputs that are *not* tensors must be passed in via `**kwargs`, and compilation will be triggered once per unique `**kwargs`.

loss_and_surrogate_loss(*model*, *guide*, **args*, ***kwargs*)

differentiable_loss(*model*, *guide*, **args*, ***kwargs*)

loss_and_grads(*model*, *guide*, **args*, ***kwargs*)

class TraceGraph_ELBO(*num_particles=1*, *max_plate_nesting=inf*, *max_iarange_nesting=None*, *vectorize_particles=False*, *strict_enumeration_warning=True*, *ignore_jit_warnings=False*, *jit_options=None*, *retain_graph=None*, *tail_adaptive_beta=-1.0*)

Bases: *pyro.infer.elbo.ELBO*

A TraceGraph implementation of ELBO-based SVI. The gradient estimator is constructed along the lines of reference [1] specialized to the case of the ELBO. It supports arbitrary dependency structure for the model and guide as well as baselines for non-reparameterizable random variables. Where possible, conditional dependency information as recorded in the `Trace` is used to reduce the variance of the gradient estimator. In particular two kinds of conditional dependency information are used to reduce variance:

- the sequential order of samples (z is sampled after y => y does not depend on z)
- `plate` generators

References

[1] ***Gradient Estimation Using Stochastic Computation Graphs***, John Schulman, Nicolas Heess, Theophane Weber, Pieter Abbeel

[2] ***Neural Variational Inference and Learning in Belief Networks*** Andriy Mnih, Karol Gregor

loss(*model*, *guide*, **args*, ***kwargs*)

Returns returns an estimate of the ELBO

Return type float

Evaluates the ELBO with an estimator that uses num_particles many samples/particles.

loss_and_grads(*model*, *guide*, **args*, ***kwargs*)

Returns returns an estimate of the ELBO

Return type float

Computes the ELBO as well as the surrogate ELBO that is used to form the gradient estimator. Performs backward on the latter. Num_particle many samples are used to form the estimators. If baselines are present, a baseline loss is also constructed and differentiated.

class JitTraceGraph_ELBO(*num_particles=1*, *max_plate_nesting=inf*, *max_iarange_nesting=None*, *vectorize_particles=False*, *strict_enumeration_warning=True*, *ignore_jit_warnings=False*, *jit_options=None*, *retain_graph=None*, *tail_adaptive_beta=-1.0*)

Bases: *pyro.infer.tracegraph_elbo.TraceGraph_ELBO*

Like *TraceGraph_ELBO* but uses `torch.jit.trace()` to compile *loss_and_grads()*.

This works only for a limited set of models:

- Models must have static structure.
- Models must not depend on any global data (except the param store).
- All model inputs that are tensors must be passed in via `*args`.
- All model inputs that are *not* tensors must be passed in via `**kwargs`, and compilation will be triggered once per unique `**kwargs`.

loss_and_grads(*model*, *guide*, **args*, ***kwargs*)

class BackwardSampleMessenger(*enum_trace*, *guide_trace*)
Bases: *pyro.poutine.messenger.Messenger*

Implements forward filtering / backward sampling for sampling from the joint posterior distribution

class TraceEnum_ELBO(*num_particles=1*, *max_plate_nesting=inf*, *max_iarange_nesting=None*, *vectorize_particles=False*, *strict_enumeration_warning=True*, *ignore_jit_warnings=False*, *jit_options=None*, *retain_graph=None*, *tail_adaptive_beta=-1.0*)
Bases: *pyro.infer.elbo.ELBO*

A trace implementation of ELBO-based SVI that supports - exhaustive enumeration over discrete sample sites, and - local parallel sampling over any sample site in the guide.

To enumerate over a sample site in the `guide`, mark the site with either `infer={'enumerate': 'sequential'}` or `infer={'enumerate': 'parallel'}`. To configure all guide sites at once, use *config_enumerate()*. To enumerate over a sample site in the `model`, mark the site `infer={'enumerate': 'parallel'}` and ensure the site does not appear in the `guide`.

This assumes restricted dependency structure on the model and guide: variables outside of an `plate` can never depend on variables inside that `plate`.

loss(*model*, *guide*, **args*, ***kwargs*)

Returns an estimate of the ELBO

Return type float

Estimates the ELBO using `num_particles` many samples (particles).

differentiable_loss(*model*, *guide*, **args*, ***kwargs*)

Returns a differentiable estimate of the ELBO

Return type torch.Tensor

Raises **ValueError** – if the ELBO is not differentiable (e.g. is identically zero)

Estimates a differentiable ELBO using `num_particles` many samples (particles). The result should be infinitely differentiable (as long as underlying derivatives have been implemented).

loss_and_grads(*model*, *guide*, **args*, ***kwargs*)

Returns an estimate of the ELBO

Return type float

Estimates the ELBO using `num_particles` many samples (particles). Performs backward on the ELBO of each particle.

compute_marginals(*model*, *guide*, **args*, ***kwargs*)
Computes marginal distributions at each model-enumerated sample site.

Returns a dict mapping site name to marginal `Distribution` object

Return type OrderedDict

sample_posterior(*model*, *guide*, **args*, ***kwargs*)
Sample from the joint posterior distribution of all model-enumerated sites given all observations

class JitTraceEnum_ELBO(*num_particles=1*, *max_plate_nesting=inf*, *max_iarange_nesting=None*, *vectorize_particles=False*, *strict_enumeration_warning=True*, *ignore_jit_warnings=False*, *jit_options=None*, *retain_graph=None*, *tail_adaptive_beta=-1.0*)
Bases: *pyro.infer.traceenum_elbo.TraceEnum_ELBO*

Like *TraceEnum_ELBO* but uses `pyro.ops.jit.compile()` to compile *loss_and_grads()*.

This works only for a limited set of models:

- Models must have static structure.
- Models must not depend on any global data (except the param store).
- All model inputs that are tensors must be passed in via `*args`.
- All model inputs that are *not* tensors must be passed in via `**kwargs`, and compilation will be triggered once per unique `**kwargs`.

differentiable_loss(*model*, *guide*, **args*, ***kwargs*)

loss_and_grads(*model*, *guide*, **args*, ***kwargs*)

class TraceMeanField_ELBO(*num_particles=1*, *max_plate_nesting=inf*, *max_iarange_nesting=None*, *vectorize_particles=False*, *strict_enumeration_warning=True*, *ignore_jit_warnings=False*, *jit_options=None*, *retain_graph=None*, *tail_adaptive_beta=-1.0*)

Bases: *pyro.infer.trace_elbo.Trace_ELBO*

A trace implementation of ELBO-based SVI. This is currently the only ELBO estimator in Pyro that uses analytic KL divergences when those are available.

In contrast to, e.g., *TraceGraph_ELBO* and `Trace_ELBO` this estimator places restrictions on the dependency structure of the model and guide. In particular it assumes that the guide has a mean-field structure, i.e. that it factorizes across the different latent variables present in the guide. It also assumes that all of the latent variables in the guide are reparameterized. This latter condition is satisfied for, e.g., the Normal distribution but is not satisfied for, e.g., the Categorical distribution.

Warning: This estimator may give incorrect results if the mean-field condition is not satisfied.

Note for advanced users:

The mean field condition is a sufficient but not necessary condition for this estimator to be correct. The precise condition is that for every latent variable z in the guide, its parents in the model must not include any latent variables that are descendants of z in the guide. Here 'parents in the model' and 'descendants in the guide' is with respect to the corresponding (statistical) dependency structure. For example, this condition is always satisfied if the model and guide have identical dependency structures.

loss(*model*, *guide*, **args*, ***kwargs*)

Returns returns an estimate of the ELBO

Return type float

Evaluates the ELBO with an estimator that uses num_particles many samples/particles.

class JitTraceMeanField_ELBO(*num_particles=1*, *max_plate_nesting=inf*, *max_iarange_nesting=None*, *vectorize_particles=False*, *strict_enumeration_warning=True*, *ignore_jit_warnings=False*, *jit_options=None*, *retain_graph=None*, *tail_adaptive_beta=-1.0*)

Bases: *pyro.infer.trace_mean_field_elbo.TraceMeanField_ELBO*

Like *TraceMeanField_ELBO* but uses *pyro.ops.jit.trace()* to compile *loss_and_grads()*.

This works only for a limited set of models:

- Models must have static structure.
- Models must not depend on any global data (except the param store).

- All model inputs that are tensors must be passed in via `*args`.
- All model inputs that are *not* tensors must be passed in via `**kwargs`, and compilation will be triggered once per unique `**kwargs`.

differentiable_loss(*model*, *guide*, **args*, ***kwargs*)

loss_and_grads(*model*, *guide*, **args*, ***kwargs*)

class TraceTailAdaptive_ELBO(*num_particles=1*, *max_plate_nesting=inf*, *max_iarange_nesting=None*, *vectorize_particles=False*, *strict_enumeration_warning=True*, *ignore_jit_warnings=False*, *jit_options=None*, *retain_graph=None*, *tail_adaptive_beta=-1.0*)

Bases: *pyro.infer.trace_elbo.Trace_ELBO*

Interface for Stochastic Variational Inference with an adaptive f-divergence as described in ref. [1]. Users should specify *num_particles* > 1 and *vectorize_particles==True*. The argument *tail_adaptive_beta* can be specified to modify how the adaptive f-divergence is constructed. See reference for details.

Note that this interface does not support computing the varational objective itself; rather it only supports computing gradients of the variational objective. Consequently, one might want to use another SVI interface (e.g. *RenyiELBO*) in order to monitor convergence.

Note that this interface only supports models in which all the latent variables are fully reparameterized. It also does not support data subsampling.

References [1] "Variational Inference with Tail-adaptive f-Divergence", Dilin Wang, Hao Liu, Qiang Liu, NeurIPS 2018 https://papers.nips.cc/paper/7816-variational-inference-with-tail-adaptive-f-divergence

loss(*model*, *guide*, **args*, ***kwargs*)

It is not necessary to estimate the tail-adaptive f-divergence itself in order to compute the corresponding gradients. Consequently the loss method is left unimplemented.

class RenyiELBO(*alpha=0*, *num_particles=2*, *max_plate_nesting=inf*, *max_iarange_nesting=None*, *vectorize_particles=False*, *strict_enumeration_warning=True*)

Bases: *pyro.infer.elbo.ELBO*

An implementation of Renyi's α-divergence variational inference following reference [1].

In order for the objective to be a strict lower bound, we require $\alpha \geq 0$. Note, however, that according to reference [1], depending on the dataset $\alpha < 0$ might give better results. In the special case $\alpha = 0$, the objective function is that of the important weighted autoencoder derived in reference [2].

Note: Setting $\alpha < 1$ gives a better bound than the usual ELBO. For $\alpha = 1$, it is better to use *Trace_ELBO* class because it helps reduce variances of gradient estimations.

Parameters

- **alpha** (*float*) – The order of α-divergence. Here $\alpha \neq 1$. Default is 0.
- **num_particles** – The number of particles/samples used to form the objective (gradient) estimator. Default is 2.
- **max_plate_nesting** (*int*) – Bound on max number of nested `pyro.plate()` contexts. Default is infinity.
- **strict_enumeration_warning** (*bool*) – Whether to warn about possible misuse of enumeration, i.e. that *TraceEnum_ELBO* is used iff there are enumerated sample sites.

References:

[1] ***Renyi Divergence Variational Inference***, Yingzhen Li, Richard E. Turner

[2] ***Importance Weighted Autoencoders***, Yuri Burda, Roger Grosse, Ruslan Salakhutdinov

loss(*model*, *guide*, **args*, ***kwargs*)

Returns returns an estimate of the ELBO

Return type float

Evaluates the ELBO with an estimator that uses num_particles many samples/particles.

loss_and_grads(*model*, *guide*, **args*, ***kwargs*)

Returns returns an estimate of the ELBO

Return type float

Computes the ELBO as well as the surrogate ELBO that is used to form the gradient estimator. Performs backward on the latter. Num_particle many samples are used to form the estimators.

class TraceTMC_ELBO(*num_particles=1*, *max_plate_nesting=inf*, *max_iarange_nesting=None*, *vectorize_particles=False*, *strict_enumeration_warning=True*, *ignore_jit_warnings=False*, *jit_options=None*, *retain_graph=None*, *tail_adaptive_beta=-1.0*)

Bases: *pyro.infer.elbo.ELBO*

A trace-based implementation of Tensor Monte Carlo [1] by way of Tensor Variable Elimination [2] that supports: - local parallel sampling over any sample site in the model or guide - exhaustive enumeration over any sample site in the model or guide

To take multiple samples, mark the site with `infer={'enumerate': 'parallel', 'num_samples': N}`. To configure all sites in a model or guide at once, use *config_enumerate()* . To enumerate or sample a sample site in the `model`, mark the site and ensure the site does not appear in the `guide`.

This assumes restricted dependency structure on the model and guide: variables outside of an `plate` can never depend on variables inside that `plate` .

References

[1] ***Tensor Monte Carlo: Particle Methods for the GPU Era***, Laurence Aitchison (2018)

[2] ***Tensor Variable Elimination for Plated Factor Graphs***, Fritz Obermeyer, Eli Bingham, Martin Jankowiak, Justin Chiu, Neeraj Pradhan, Alexander Rush, Noah Goodman (2019)

differentiable_loss(*model*, *guide*, **args*, ***kwargs*)

Returns a differentiable estimate of the marginal log-likelihood

Return type torch.Tensor

Raises **ValueError** – if the ELBO is not differentiable (e.g. is identically zero)

Computes a differentiable TMC estimate using `num_particles` many samples (particles). The result should be infinitely differentiable (as long as underlying derivatives have been implemented).

loss(*model*, *guide*, **args*, ***kwargs*)

loss_and_grads(*model*, *guide*, **args*, ***kwargs*)

3.3 Importance

class Importance(*model*, *guide=None*, *num_samples=None*)
Bases: *pyro.infer.abstract_infer.TracePosterior*

Parameters

- **model** – probabilistic model defined as a function
- **guide** – guide used for sampling defined as a function
- **num_samples** – number of samples to draw from the guide (default 10)

This method performs posterior inference by importance sampling using the guide as the proposal distribution. If no guide is provided, it defaults to proposing from the model's prior.

get_ESS()
Compute (Importance Sampling) Effective Sample Size (ESS).

get_log_normalizer()
Estimator of the normalizing constant of the target distribution. (mean of the unnormalized weights)

get_normalized_weights(*log_scale=False*)
Compute the normalized importance weights.

psis_diagnostic(*model*, *guide*, **args*, ***kwargs*)
Computes the Pareto tail index k for a model/guide pair using the technique described in [1], which builds on previous work in [2]. If $0 < k < 0.5$ the guide is a good approximation to the model posterior, in the sense described in [1]. If $0.5 \leq k \leq 0.7$, the guide provides a suboptimal approximation to the posterior, but may still be useful in practice. If $k > 0.7$ the guide program provides a poor approximation to the full posterior, and caution should be used when using the guide. Note, however, that a guide may be a poor fit to the full posterior while still yielding reasonable model predictions. If $k < 0.0$ the importance weights corresponding to the model and guide appear to be bounded from above; this would be a bizarre outcome for a guide trained via ELBO maximization. Please see [1] for a more complete discussion of how the tail index k should be interpreted.

Please be advised that a large number of samples may be required for an accurate estimate of k.

Note that we assume that the model and guide are both vectorized and have static structure. As is canonical in Pyro, the args and kwargs are passed to the model and guide.

References [1] 'Yes, but Did It Work?: Evaluating Variational Inference.' Yuling Yao, Aki Vehtari, Daniel Simpson, Andrew Gelman [2] 'Pareto Smoothed Importance Sampling.' Aki Vehtari, Andrew Gelman, Jonah Gabry

Parameters

- **model** (*callable*) – the model program.
- **guide** (*callable*) – the guide program.
- **num_particles** (*int*) – the total number of times we run the model and guide in order to compute the diagnostic. defaults to 1000.
- **max_simultaneous_particles** – the maximum number of simultaneous samples drawn from the model and guide. defaults to *num_particles*. *num_particles* must be divisible by *max_simultaneous_particles*. compute the diagnostic. defaults to 1000.
- **max_plate_nesting** (*int*) – optional bound on max number of nested `pyro.plate()` contexts in the model/guide. defaults to 7.

Returns float the PSIS diagnostic k

vectorized_importance_weights(*model*, *guide*, **args*, ***kwargs*)

Parameters

- **model** – probabilistic model defined as a function
- **guide** – guide used for sampling defined as a function
- **num_samples** – number of samples to draw from the guide (default 1)
- **max_plate_nesting** (*int*) – Bound on max number of nested `pyro.plate()` contexts.
- **normalized** (*bool*) – set to True to return self-normalized importance weights

Returns returns a `(num_samples,)`-shaped tensor of importance weights and the model and guide traces that produced them

Vectorized computation of importance weights for models with static structure:

```
log_weights, model_trace, guide_trace = \
    vectorized_importance_weights(model, guide, *args,
                                  num_samples=1000,
                                  max_plate_nesting=4,
                                  normalized=False)
```

3.4 Reweighted Wake-Sleep

class ReweightedWakeSleep(*num_particles=2*, *insomnia=1.0*, *model_has_params=True*, *num_sleep_particles=None*, *vectorize_particles=True*, *max_plate_nesting=inf*, *strict_enumeration_warning=True*)

Bases: *pyro.infer.elbo.ELBO*

An implementation of Reweighted Wake Sleep following reference [1].

Note: Sampling and log_prob evaluation asymptotic complexity:

---

1) **Using wake-theta and/or wake-phi** O(*num_particles*) samples from guide, O(*num_particles*) *log_prob* evaluations of model and guide
2) **Using sleep-phi** O(*num_sleep_particles*) samples from model, O(*num_sleep_particles*) *log_prob* evaluations of guide

if 1) and 2) are combined, O(*num_particles*) samples from the guide, O(*num_sleep_particles*) from the model, O(*num_particles* + *num_sleep_particles*) *log_prob* evaluations of the guide, and O(*num_particles*) evaluations of the model

---

Note: This is particularly useful for models with stochastic branching, as described in [2].

Note: This returns _two_ losses, one each for (a) the model parameters (*theta*), computed using the *iwae* objective, and (b) the guide parameters (*phi*), computed using (a combination of) the *csis* objective and a self-normalized importance-sampled version of the *csis* objective.

Note: In order to enable computing the sleep-phi terms, the guide program must have its observations explicitly passed in through the keyworded argument *observations*. Where the value of the observations is unknown during definition, such as for amortized variational inference, it may be given a default argument as *observations=None*, and the correct value supplied during learning through *svi.step(observations=...)*.

Warning: Mini-batch training is not supported yet.

Parameters

- **num_particles** (*int*) – The number of particles/samples used to form the objective (gradient) estimator. Default is 2.
- **insomnia** – The scaling between the wake-phi and sleep-phi terms. Default is 1.0 [wake-phi]
- **model_has_params** (*bool*) – Indicate if model has learnable params. Useful in avoiding extra computation when running in pure sleep mode [csis]. Default is True.
- **num_sleep_particles** (*int*) – The number of particles used to form the sleep-phi estimator. Matches *num_particles* by default.
- **vectorize_particles** (*bool*) – Whether the traces should be vectorised across *num_particles*. Default is True.
- **max_plate_nesting** (*int*) – Bound on max number of nested `pyro.plate()` contexts. Default is infinity.
- **strict_enumeration_warning** (*bool*) – Whether to warn about possible misuse of enumeration, i.e. that *TraceEnum_ELBO* is used iff there are enumerated sample sites.

References:

[1] ***Reweighted Wake-Sleep***, Jörg Bornschein, Yoshua Bengio

[2] ***Revisiting Reweighted Wake-Sleep for Models with Stochastic Control Flow***, Tuan Anh Le, Adam R. Kosiorek, N. Siddharth, Yee Whye Teh, Frank Wood

loss(*model*, *guide*, **args*, ***kwargs*)

Returns returns model loss and guide loss

Return type float, float

Computes the re-weighted wake-sleep estimators for the model (wake-theta) and the guide (insomnia * wake-phi + (1 - insomnia) * sleep-phi).

loss_and_grads(*model*, *guide*, **args*, ***kwargs*)

Returns returns model loss and guide loss

Return type float

Computes the RWS estimators for the model (wake-theta) and the guide (wake-phi). Performs backward as appropriate on both, using num_particle many samples/particles.

3.5 Sequential Monte Carlo

exception SMCFailed
Bases: ValueError

Exception raised when *SMCFilter* fails to find any hypothesis with nonzero probability.

class SMCFilter(*model*, *guide*, *num_particles*, *max_plate_nesting*, *, *ess_threshold=0.5*)
Bases: object

SMCFilter is the top-level interface for filtering via sequential monte carlo.

The model and guide should be objects with two methods: `.init(state, ...)` and `.step(state, ...)`, intended to be called first with *init()* , then with *step()* repeatedly. These two methods should have the same signature as *SMCFilter* 's *init()* and *step()* of this class, but with an extra first argument `state` that should be used to store all tensors that depend on sampled variables. The `state` will be a dict-like object, *SMCState* , with arbitrary keys and `torch.Tensor` values. Models can read and write `state` but guides can only read from it.

Inference complexity is `O(len(state) * num_time_steps)`, so to avoid quadratic complexity in Markov models, ensure that `state` has fixed size.

Parameters

- **model** (*object*) – probabilistic model with `init` and `step` methods
- **guide** (*object*) – guide used for sampling, with `init` and `step` methods
- **num_particles** (*int*) – The number of particles used to form the distribution.
- **max_plate_nesting** (*int*) – Bound on max number of nested `pyro.plate()` contexts.
- **ess_threshold** (*float*) – Effective sample size threshold for deciding when to importance resample: resampling occurs when `ess < ess_threshold * num_particles`.

get_empirical()

Returns a marginal distribution over all state tensors.

Return type a dictionary with keys which are latent variables and values which are *Empirical* objects.

init(**args*, ***kwargs*)
Perform any initialization for sequential importance resampling. Any args or kwargs are passed to the model and guide

step(**args*, ***kwargs*)
Take a filtering step using sequential importance resampling updating the particle weights and values while resampling if desired. Any args or kwargs are passed to the model and guide

class SMCState(*num_particles*)
Bases: dict

Dictionary-like object to hold a vectorized collection of tensors to represent all state during inference with *SMCFilter*. During inference, the *SMCFilter* resample these tensors.

Keys may have arbitrary hashable type. Values must be `torch.Tensor` s.

Parameters **num_particles** (*int*) –

3.6 Stein Methods

class IMQSteinKernel(*alpha=0.5*, *beta=-0.5*, *bandwidth_factor=None*)
Bases: *pyro.infer.svgd.SteinKernel*

An IMQ (inverse multi-quadratic) kernel for use in the SVGD inference algorithm [1]. The bandwidth of the kernel is chosen from the particles using a simple heuristic as in reference [2]. The kernel takes the form

$K(x, y) = (\alpha + ||x - y||^2/h)^\beta$

where α and β are user-specified parameters and h is the bandwidth.

Parameters

- **alpha** (*float*) – Kernel hyperparameter, defaults to 0.5.
- **beta** (*float*) – Kernel hyperparameter, defaults to -0.5.
- **bandwidth_factor** (*float*) – Optional factor by which to scale the bandwidth, defaults to 1.0.

Variables **bandwidth_factor** (*float*) – Property that controls the factor by which to scale the bandwidth at each iteration.

References

[1] "Stein Points," Wilson Ye Chen, Lester Mackey, Jackson Gorham, Francois-Xavier Briol, Chris. J. Oates.
[2] "Stein Variational Gradient Descent: A General Purpose Bayesian Inference Algorithm," Qiang Liu, Dilin Wang

bandwidth_factor

log_kernel_and_grad(*particles*)
See *pyro.infer.svgd.SteinKernel.log_kernel_and_grad()*

class RBFSteinKernel(*bandwidth_factor=None*)
Bases: *pyro.infer.svgd.SteinKernel*

A RBF kernel for use in the SVGD inference algorithm. The bandwidth of the kernel is chosen from the particles using a simple heuristic as in reference [1].

Parameters **bandwidth_factor** (*float*) – Optional factor by which to scale the bandwidth, defaults to 1.0.

Variables **bandwidth_factor** (*float*) – Property that controls the factor by which to scale the bandwidth at each iteration.

References

[1] "Stein Variational Gradient Descent: A General Purpose Bayesian Inference Algorithm," Qiang Liu, Dilin Wang

bandwidth_factor

log_kernel_and_grad(*particles*)
See *pyro.infer.svgd.SteinKernel.log_kernel_and_grad()*

class SVGD(*model*, *kernel*, *optim*, *num_particles*, *max_plate_nesting*, *mode='univariate'*)
Bases: object

A basic implementation of Stein Variational Gradient Descent as described in reference [1].

Parameters

- **model** – The model (callable containing Pyro primitives). Model must be fully vectorized and may only contain continuous latent variables.
- **kernel** – a SVGD compatible kernel like *RBFSteinKernel*.
- **optim** (*pyro.optim.PyroOptim*) – A wrapper for a PyTorch optimizer.
- **num_particles** (*int*) – The number of particles used in SVGD.
- **max_plate_nesting** (*int*) – The max number of nested `pyro.plate()` contexts in the model.
- **mode** (*str*) – Whether to use a Kernelized Stein Discrepancy that makes use of *multivariate* test functions (as in [1]) or *univariate* test functions (as in [2]). Defaults to *univariate*.

Example usage:

```
from pyro.infer import SVGD, RBFSteinKernel
from pyro.optim import Adam

kernel = RBFSteinKernel()
adam = Adam({"lr": 0.1})
svgd = SVGD(model, kernel, adam, num_particles=50, max_plate_nesting=0)

for step in range(500):
    svgd.step(model_arg1, model_arg2)

final_particles = svgd.get_named_particles()
```

References

[1] "Stein Variational Gradient Descent: A General Purpose Bayesian Inference Algorithm," Qiang Liu, Dilin Wang

[2] "Kernelized Complete Conditional Stein Discrepancy," Raghav Singhal, Saad Lahlou, Rajesh Ranganath

get_named_particles()
Create a dictionary mapping name to vectorized value, of the form `{name: tensor}`. The leading dimension of each tensor corresponds to particles, i.e. this creates a struct of arrays.

step(**args*, ***kwargs*)
Computes the SVGD gradient, passing args and kwargs to the model, and takes a gradient step.

Return dict A dictionary of the form {name: float}, where each float is a mean squared gradient. This can be used to monitor the convergence of SVGD.

class SteinKernel
Bases: `object`

Abstract class for kernels used in the *SVGD* inference algorithm.

log_kernel_and_grad(*particles*)
Compute the component kernels and their gradients.

Parameters **particles** – a tensor with shape (N, D)

Returns A pair (*log_kernel*, *kernel_grad*) where *log_kernel* is a (N, N, D)-shaped tensor equal to the logarithm of the kernel and *kernel_grad* is a (N, N, D)-shaped tensor where the entry (n, m, d) represents the derivative of *log_kernel* w.r.t. x_{m,d}, where x_{m,d} is the d^th dimension of particle m.

vectorize(*fn*, *num_particles*, *max_plate_nesting*)

3.7 Likelihood free methods

class EnergyDistance(*beta=1.0*, *prior_scale=0.0*, *num_particles=2*, *max_plate_nesting=inf*)
Bases: object

Posterior predictive energy distance [1,2] with optional Bayesian regularization by the prior.

Let *p(x,z)=p(z) p(x|z)* be the model, *q(z|x)* be the guide. Then given data *x* and drawing an iid pair of samples (Z, X) and (Z', X') (where *Z* is latent and *X* is the posterior predictive),

$$
\begin{aligned}
&Z \sim q(z|x); \quad X \sim p(x|Z) \\
&Z' \sim q(z|x); \quad X' \sim p(x|Z') \\
&loss = \mathbb{E}_X \|X - x\|^\beta - \frac{1}{2}\mathbb{E}_{X,X'} \|X - X'\|^\beta - \lambda \mathbb{E}_Z \log p(Z)
\end{aligned}
$$

This is a likelihood-free inference algorithm, and can be used for likelihoods without tractable density functions. The β energy distance is a robust loss functions, and is well defined for any distribution with finite fractional moment $\mathbb{E}[\|X\|^\beta]$.

This requires static model structure, a fully reparametrized guide, and reparametrized likelihood distributions in the model. Model latent distributions may be non-reparametrized.

References

[1] Gabor J. Szekely, Maria L. Rizzo (2003) Energy Statistics: A Class of Statistics Based on Distances.

[2] Tilmann Gneiting, Adrian E. Raftery (2007) Strictly Proper Scoring Rules, Prediction, and Estimation. https://www.stat.washington.edu/raftery/Research/PDF/Gneiting2007jasa.pdf

Parameters

- **beta** (*float*) – Exponent β from [1,2]. The loss function is strictly proper for distributions with finite *beta*-absolute moment $E[\|X\|^\beta]$. Thus for heavy tailed distributions `beta` should be small, e.g. for `Cauchy` distributions, $\beta < 1$ is strictly proper. Defaults to 1. Must be in the open interval (0,2).
- **prior_scale** (*float*) – Nonnegative scale for prior regularization. Model parameters are trained only if this is positive. If zero (default), then model log densities will not be computed (guide log densities are never computed).
- **num_particles** (*int*) – The number of particles/samples used to form the gradient estimators. Must be at least 2.
- **max_plate_nesting** (*int*) – Optional bound on max number of nested `pyro.plate()` contexts. If omitted, this will guess a valid value by running the (model,guide) pair once.

__call__(*model*, *guide*, **args*, ***kwargs*)
Computes the surrogate loss that can be differentiated with autograd to produce gradient estimates for the model and guide parameters.

loss(**args*, ***kwargs*)
Not implemented. Added for compatibility with unit tests only.

3.8 Discrete Inference

infer_discrete(*fn=None*, *first_available_dim=None*, *temperature=1*, ***, *strict_enumeration_warning=True*)

A poutine that samples discrete sites marked with `site["infer"]["enumerate"] = "parallel"` from the posterior, conditioned on observations.

Example:

```
@infer_discrete(first_available_dim=-1, temperature=0)
@config_enumerate
def viterbi_decoder(data, hidden_dim=10):
    transition = 0.3 / hidden_dim + 0.7 * torch.eye(hidden_dim)
    means = torch.arange(float(hidden_dim))
    states = [0]
    for t in pyro.markov(range(len(data))):
        states.append(pyro.sample("states_{}".format(t),
                                  dist.Categorical(transition[states[-1]])))
        pyro.sample("obs_{}".format(t),
                    dist.Normal(means[states[-1]], 1.),
                    obs=data[t])
    return states  # returns maximum likelihood states
```

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls)
- **first_available_dim** (*int*) – The first tensor dimension (counting from the right) that is available for parallel enumeration. This dimension and all dimensions left may be used internally by Pyro. This should be a negative integer.
- **temperature** (*int*) – Either 1 (sample via forward-filter backward-sample) or 0 (optimize via Viterbi-like MAP inference). Defaults to 1 (sample).
- **strict_enumeration_warning** (*bool*) – Whether to warn in case no enumerated sample sites are found. Defalts to True.

class TraceEnumSample_ELBO(*num_particles=1*, *max_plate_nesting=inf*, *max_iarange_nesting=None*, *vectorize_particles=False*, *strict_enumeration_warning=True*, *ignore_jit_warnings=False*, *jit_options=None*, *retain_graph=None*, *tail_adaptive_beta=-1.0*)

Bases: *pyro.infer.traceenum_elbo.TraceEnum_ELBO*

This extends `TraceEnum_ELBO` to make it cheaper to sample from discrete latent states during SVI.

The following are equivalent but the first is cheaper, sharing work between the computations of `loss` and `z`:

```
# Version 1.
elbo = TraceEnumSample_ELBO(max_plate_nesting=1)
loss = elbo.loss(*args, **kwargs)
z = elbo.sample_saved()

# Version 2.
elbo = TraceEnum_ELBO(max_plate_nesting=1)
loss = elbo.loss(*args, **kwargs)
guide_trace = poutine.trace(guide).get_trace(*args, **kwargs)
z = infer_discrete(poutine.replay(model, guide_trace),
                   first_available_dim=-2)(*args, **kwargs)
```

sample_saved()
Generate latent samples while reusing work from SVI.step().

3.9 Inference Utilities

class Predictive(*model*, *posterior_samples=None*, *guide=None*, *num_samples=None*, *return_sites=()*, *parallel=False*)
Bases: torch.nn.modules.module.Module

EXPERIMENTAL class used to construct predictive distribution. The predictive distribution is obtained by running the *model* conditioned on latent samples from *posterior_samples*. If a *guide* is provided, then posterior samples from all the latent sites are also returned.

Warning: The interface for the *Predictive* class is experimental, and might change in the future.

Parameters

- **model** – Python callable containing Pyro primitives.
- **posterior_samples** (*dict*) – dictionary of samples from the posterior.
- **guide** (*callable*) – optional guide to get posterior samples of sites not present in *posterior_samples*.
- **num_samples** (*int*) – number of samples to draw from the predictive distribution. This argument has no effect if posterior_samples is non-empty, in which case, the leading dimension size of samples in posterior_samples is used.
- **return_sites** (*list, tuple, or set*) – sites to return; by default only sample sites not present in *posterior_samples* are returned.
- **parallel** (*bool*) – predict in parallel by wrapping the existing model in an outermost *plate* messenger. Note that this requires that the model has all batch dims correctly annotated via plate. Default is *False*.

call(**args*, ***kwargs*)
Method that calls *forward()* and returns parameter values of the guide as a *tuple* instead of a *dict*, which is a requirement for JIT tracing. Unlike *forward()*, this method can be traced by torch.jit.trace_module().

Warning: This method may be removed once PyTorch JIT tracer starts accepting *dict* as valid return types. See issue.

forward(**args*, ***kwargs*)
Returns dict of samples from the predictive distribution. By default, only sample sites not contained in *posterior_samples* are returned. This can be modified by changing the *return_sites* keyword argument of this *Predictive* instance.

Note: This method is used internally by Module. Users should instead use __call__() as in Predictive(model)(*args, **kwargs).

Parameters

- **args** – model arguments.
- **kwargs** – model keyword arguments.

get_samples(**args*, ***kwargs*)

get_vectorized_trace(**args*, ***kwargs*)

Returns a single vectorized *trace* from the predictive distribution. Note that this requires that the model has all batch dims correctly annotated via `plate`.

Parameters

- **args** – model arguments.
- **kwargs** – model keyword arguments.

class EmpiricalMarginal(*trace_posterior*, *sites=None*, *validate_args=None*)

Bases: `pyro.distributions.empirical.Empirical`

Marginal distribution over a single site (or multiple, provided they have the same shape) from the `TracePosterior`'s model.

Note: If multiple sites are specified, they must have the same tensor shape. Samples from each site will be stacked and stored within a single tensor. See *Empirical*. To hold the marginal distribution of sites having different shapes, use *Marginals* instead.

Parameters

- **trace_posterior** (TracePosterior) – a `TracePosterior` instance representing a Monte Carlo posterior.
- **sites** (*list*) – optional list of sites for which we need to generate the marginal distribution.

class Marginals(*trace_posterior*, *sites=None*, *validate_args=None*)

Bases: `object`

Holds the marginal distribution over one or more sites from the `TracePosterior`'s model. This is a convenience container class, which can be extended by `TracePosterior` subclasses. e.g. for implementing diagnostics.

Parameters

- **trace_posterior** (TracePosterior) – a TracePosterior instance representing a Monte Carlo posterior.
- **sites** (*list*) – optional list of sites for which we need to generate the marginal distribution.

empirical

A dictionary of sites' names and their corresponding *EmpiricalMarginal* distribution.

Type `OrderedDict`

support(*flatten=False*)

Gets support of this marginal distribution.

Parameters **flatten** (*bool*) – A flag to decide if we want to flatten *batch_shape* when the marginal distribution is collected from the posterior with `num_chains > 1`. Defaults to False.

Returns a dict with keys are sites' names and values are sites' supports.

Return type `OrderedDict`

class TracePosterior(*num_chains=1*)
Bases: `object`

Abstract TracePosterior object from which posterior inference algorithms inherit. When run, collects a bag of execution traces from the approximate posterior. This is designed to be used by other utility classes like *EmpiricalMarginal*, that need access to the collected execution traces.

information_criterion(*pointwise=False*)
Computes information criterion of the model. Currently, returns only "Widely Applicable/Watanabe-Akaike Information Criterion" (WAIC) and the corresponding effective number of parameters.

Reference:

[1] *Practical Bayesian model evaluation using leave-one-out cross-validation and WAIC*, Aki Vehtari, Andrew Gelman, and Jonah Gabry

Parameters **pointwise** (*bool*) – a flag to decide if we want to get a vectorized WAIC or not. When `pointwise=False`, returns the sum.

Returns a dictionary containing values of WAIC and its effective number of parameters.

Return type `OrderedDict`

marginal(*sites=None*)
Generates the marginal distribution of this posterior.

Parameters **sites** (*list*) – optional list of sites for which we need to generate the marginal distribution.

Returns A *Marginals* class instance.

Return type *Marginals*

run(**args*, ***kwargs*)
Calls *self._traces* to populate execution traces from a stochastic Pyro model.

Parameters

- **args** – optional args taken by *self._traces*.
- **kwargs** – optional keywords args taken by *self._traces*.

class TracePredictive(*model*, *posterior*, *num_samples*, *keep_sites=None*)
Bases: *pyro.infer.abstract_infer.TracePosterior*

> **Warning:** This class is deprecated and will be removed in a future release. Use the *Predictive* class instead.

Generates and holds traces from the posterior predictive distribution, given model execution traces from the approximate posterior. This is achieved by constraining latent sites to randomly sampled parameter values from the model execution traces and running the model forward to generate traces with new response ("_RETURN") sites. :param model: arbitrary Python callable containing Pyro primitives. :param TracePosterior posterior: trace posterior instance holding samples from the model's approximate posterior. :param int num_samples: number of samples to generate. :param keep_sites: The sites which should be sampled from posterior distribution (default: all)

marginal(*sites=None*)
Gets marginal distribution for this predictive posterior distribution.

3.10 MCMC

3.10.1 MCMC

class MCMC(*kernel*, *num_samples*, *warmup_steps=None*, *initial_params=None*, *num_chains=1*, *hook_fn=None*, *mp_context=None*, *disable_progbar=False*, *disable_validation=True*, *transforms=None*)

Bases: `object`

Wrapper class for Markov Chain Monte Carlo algorithms. Specific MCMC algorithms are TraceKernel instances and need to be supplied as a `kernel` argument to the constructor.

Note: The case of *num_chains > 1* uses python multiprocessing to run parallel chains in multiple processes. This goes with the usual caveats around multiprocessing in python, e.g. the model used to initialize the `kernel` must be serializable via *pickle*, and the performance / constraints will be platform dependent (e.g. only the "spawn" context is available in Windows). This has also not been extensively tested on the Windows platform.

Parameters

- **kernel** – An instance of the `TraceKernel` class, which when given an execution trace returns another sample trace from the target (posterior) distribution.
- **num_samples** (*int*) – The number of samples that need to be generated, excluding the samples discarded during the warmup phase.
- **warmup_steps** (*int*) – Number of warmup iterations. The samples generated during the warmup phase are discarded. If not provided, default is is the same as *num_samples*.
- **num_chains** (*int*) – Number of MCMC chains to run in parallel. Depending on whether *num_chains* is 1 or more than 1, this class internally dispatches to either *_UnarySampler* or *_MultiSampler*.
- **initial_params** (*dict*) – dict containing initial tensors in unconstrained space to initiate the markov chain. The leading dimension's size must match that of *num_chains*. If not specified, parameter values will be sampled from the prior.
- **hook_fn** – Python callable that takes in *(kernel, samples, stage, i)* as arguments. stage is either *sample* or *warmup* and i refers to the i'th sample for the given stage. This can be used to implement additional logging, or more generally, run arbitrary code per generated sample.
- **mp_context** (*str*) – Multiprocessing context to use when *num_chains > 1*. Only applicable for Python 3.5 and above. Use *mp_context="spawn"* for CUDA.
- **disable_progbar** (*bool*) – Disable progress bar and diagnostics update.
- **disable_validation** (*bool*) – Disables distribution validation check. Defaults to `True`, disabling validation, since divergent transitions will lead to exceptions. Switch to `False` to enable validation, or to `None` to preserve existing global values.
- **transforms** (*dict*) – dictionary that specifies a transform for a sample site with constrained support to unconstrained space.

diagnostics()

Gets some diagnostics statistics such as effective sample size, split Gelman-Rubin, or divergent transitions from the sampler.

get_samples(*num_samples=None*, *group_by_chain=False*)
Get samples from the MCMC run, potentially resampling with replacement.

Parameters

- **num_samples** (*int*) – Number of samples to return. If *None*, all the samples from an MCMC chain are returned in their original ordering.
- **group_by_chain** (*bool*) – Whether to preserve the chain dimension. If True, all samples will have num_chains as the size of their leading dimension.

Returns dictionary of samples keyed by site name.

run
Run MCMC to generate samples and populate *self._samples*.

Example usage:

```
def model(data):
    ...

nuts_kernel = NUTS(model)
mcmc = MCMC(nuts_kernel, num_samples=500)
mcmc.run(data)
samples = mcmc.get_samples()
```

Parameters

- **args** – optional arguments taken by *MCMCKernel.setup*.
- **kwargs** – optional keywords arguments taken by *MCMCKernel.setup*.

summary(*prob=0.9*)
Prints a summary table displaying diagnostics of samples obtained from posterior. The diagnostics displayed are mean, standard deviation, median, the 90% Credibility Interval, *effective_sample_size()*, *split_gelman_rubin()*.

Parameters **prob** (*float*) – the probability mass of samples within the credibility interval.

3.10.2 MCMCKernel

class MCMCKernel
Bases: object

cleanup()
Optional method to clean up any residual state on termination.

diagnostics()
Returns a dict of useful diagnostics after finishing sampling process.

end_warmup()
Optional method to tell kernel that warm-up phase has been finished.

initial_params
Returns a dict of initial params (by default, from the prior) to initiate the MCMC run.

Returns dict of parameter values keyed by their name.

logging()
Relevant logging information to be printed at regular intervals of the MCMC run. Returns *None* by default.

Returns String containing the diagnostic summary. e.g. acceptance rate

Return type string

sample(*params*)
Samples parameters from the posterior distribution, when given existing parameters.

Parameters

- **params** (*dict*) – Current parameter values.
- **time_step** (*int*) – Current time step.

Returns New parameters from the posterior distribution.

setup(*warmup_steps*, **args*, ***kwargs*)
Optional method to set up any state required at the start of the simulation run.

Parameters

- **warmup_steps** (*int*) – Number of warmup iterations.
- ***args** – Algorithm specific positional arguments.
- ****kwargs** – Algorithm specific keyword arguments.

3.10.3 HMC

class HMC(*model=None*, *potential_fn=None*, *step_size=1*, *trajectory_length=None*, *num_steps=None*, *adapt_step_size=True*, *adapt_mass_matrix=True*, *full_mass=False*, *transforms=None*, *max_plate_nesting=None*, *jit_compile=False*, *jit_options=None*, *ignore_jit_warnings=False*, *target_accept_prob=0.8*, *init_strategy=<function init_to_uniform>*)
Bases: *pyro.infer.mcmc.mcmc_kernel.MCMCKernel*

Simple Hamiltonian Monte Carlo kernel, where `step_size` and `num_steps` need to be explicitly specified by the user.

References

[1] *MCMC Using Hamiltonian Dynamics*, Radford M. Neal

Parameters

- **model** – Python callable containing Pyro primitives.
- **potential_fn** – Python callable calculating potential energy with input is a dict of real support parameters.
- **step_size** (*float*) – Determines the size of a single step taken by the verlet integrator while computing the trajectory using Hamiltonian dynamics. If not specified, it will be set to 1.
- **trajectory_length** (*float*) – Length of a MCMC trajectory. If not specified, it will be set to `step_size x num_steps`. In case `num_steps` is not specified, it will be set to 2π.
- **num_steps** (*int*) – The number of discrete steps over which to simulate Hamiltonian dynamics. The state at the end of the trajectory is returned as the proposal. This value is always equal to `int(trajectory_length / step_size)`.
- **adapt_step_size** (*bool*) – A flag to decide if we want to adapt step_size during warm-up phase using Dual Averaging scheme.

- **adapt_mass_matrix** (*bool*) – A flag to decide if we want to adapt mass matrix during warm-up phase using Welford scheme.
- **full_mass** (*bool*) – A flag to decide if mass matrix is dense or diagonal.
- **transforms** (*dict*) – Optional dictionary that specifies a transform for a sample site with constrained support to unconstrained space. The transform should be invertible, and implement *log_abs_det_jacobian*. If not specified and the model has sites with constrained support, automatic transformations will be applied, as specified in `torch.distributions.constraint_registry`.
- **max_plate_nesting** (*int*) – Optional bound on max number of nested `pyro.plate()` contexts. This is required if model contains discrete sample sites that can be enumerated over in parallel.
- **jit_compile** (*bool*) – Optional parameter denoting whether to use the PyTorch JIT to trace the log density computation, and use this optimized executable trace in the integrator.
- **jit_options** (*dict*) – A dictionary contains optional arguments for `torch.jit.trace()` function.
- **ignore_jit_warnings** (*bool*) – Flag to ignore warnings from the JIT tracer when `jit_compile=True`. Default is False.
- **target_accept_prob** (*float*) – Increasing this value will lead to a smaller step size, hence the sampling will be slower and more robust. Default to 0.8.
- **init_strategy** (*callable*) – A per-site initialization function. See *Initialization* section for available functions.

Note: Internally, the mass matrix will be ordered according to the order of the names of latent variables, not the order of their appearance in the model.

Example:

```
>>> true_coefs = torch.tensor([1., 2., 3.])
>>> data = torch.randn(2000, 3)
>>> dim = 3
>>> labels = dist.Bernoulli(logits=(true_coefs * data).sum(-1)).sample()
>>>
>>> def model(data):
...     coefs_mean = torch.zeros(dim)
...     coefs = pyro.sample('beta', dist.Normal(coefs_mean, torch.ones(3)))
...     y = pyro.sample('y', dist.Bernoulli(logits=(coefs * data).sum(-1)),␣
↪obs=labels)
...     return y
>>>
>>> hmc_kernel = HMC(model, step_size=0.0855, num_steps=4)
>>> mcmc = MCMC(hmc_kernel, num_samples=500, warmup_steps=100)
>>> mcmc.run(data)
>>> mcmc.get_samples()['beta'].mean(0)  # doctest: +SKIP
tensor([ 0.9819,  1.9258,  2.9737])
```

cleanup()

clear_cache()

diagnostics()

initial_params

inverse_mass_matrix

logging()

mass_matrix_adapter

num_steps

sample(*params*)

setup(*warmup_steps*, **args*, ***kwargs*)

step_size

3.10.4 NUTS

class NUTS(*model=None*, *potential_fn=None*, *step_size=1*, *adapt_step_size=True*, *adapt_mass_matrix=True*, *full_mass=False*, *use_multinomial_sampling=True*, *transforms=None*, *max_plate_nesting=None*, *jit_compile=False*, *jit_options=None*, *ignore_jit_warnings=False*, *target_accept_prob=0.8*, *max_tree_depth=10*, *init_strategy=<function init_to_uniform>*)

Bases: pyro.infer.mcmc.hmc.HMC

No-U-Turn Sampler kernel, which provides an efficient and convenient way to run Hamiltonian Monte Carlo. The number of steps taken by the integrator is dynamically adjusted on each call to `sample` to ensure an optimal length for the Hamiltonian trajectory [1]. As such, the samples generated will typically have lower autocorrelation than those generated by the *HMC* kernel. Optionally, the NUTS kernel also provides the ability to adapt step size during the warmup phase.

Refer to the baseball example to see how to do Bayesian inference in Pyro using NUTS.

References

[1] ***The No-U-turn sampler: adaptively setting path lengths in Hamiltonian Monte Carlo*,** Matthew D. Hoffman, and Andrew Gelman.

[2] ***A Conceptual Introduction to Hamiltonian Monte Carlo*,** Michael Betancourt

[3] ***Slice Sampling*,** Radford M. Neal

Parameters

- **model** – Python callable containing Pyro primitives.
- **potential_fn** – Python callable calculating potential energy with input is a dict of real support parameters.
- **step_size** (*float*) – Determines the size of a single step taken by the verlet integrator while computing the trajectory using Hamiltonian dynamics. If not specified, it will be set to 1.
- **adapt_step_size** (*bool*) – A flag to decide if we want to adapt step_size during warm-up phase using Dual Averaging scheme.
- **adapt_mass_matrix** (*bool*) – A flag to decide if we want to adapt mass matrix during warm-up phase using Welford scheme.
- **full_mass** (*bool*) – A flag to decide if mass matrix is dense or diagonal.
- **use_multinomial_sampling** (*bool*) – A flag to decide if we want to sample candidates along its trajectory using "multinomial sampling" or using "slice sampling". Slice sampling is used in the original NUTS paper [1], while multinomial sampling is suggested in [2]. By default, this flag is set to True. If it is set to *False*, NUTS uses slice sampling.

- **transforms** (*dict*) – Optional dictionary that specifies a transform for a sample site with constrained support to unconstrained space. The transform should be invertible, and implement *log_abs_det_jacobian*. If not specified and the model has sites with constrained support, automatic transformations will be applied, as specified in `torch.distributions.constraint_registry`.
- **max_plate_nesting** (*int*) – Optional bound on max number of nested `pyro.plate()` contexts. This is required if model contains discrete sample sites that can be enumerated over in parallel.
- **jit_compile** (*bool*) – Optional parameter denoting whether to use the PyTorch JIT to trace the log density computation, and use this optimized executable trace in the integrator.
- **jit_options** (*dict*) – A dictionary contains optional arguments for `torch.jit.trace()` function.
- **ignore_jit_warnings** (*bool*) – Flag to ignore warnings from the JIT tracer when `jit_compile=True`. Default is False.
- **target_accept_prob** (*float*) – Target acceptance probability of step size adaptation scheme. Increasing this value will lead to a smaller step size, so the sampling will be slower but more robust. Default to 0.8.
- **max_tree_depth** (*int*) – Max depth of the binary tree created during the doubling scheme of NUTS sampler. Default to 10.
- **init_strategy** (*callable*) – A per-site initialization function. See *Initialization* section for available functions.

Example:

```
>>> true_coefs = torch.tensor([1., 2., 3.])
>>> data = torch.randn(2000, 3)
>>> dim = 3
>>> labels = dist.Bernoulli(logits=(true_coefs * data).sum(-1)).sample()
>>>
>>> def model(data):
...     coefs_mean = torch.zeros(dim)
...     coefs = pyro.sample('beta', dist.Normal(coefs_mean, torch.ones(3)))
...     y = pyro.sample('y', dist.Bernoulli(logits=(coefs * data).sum(-1)),␣
↪obs=labels)
...     return y
>>>
>>> nuts_kernel = NUTS(model, adapt_step_size=True)
>>> mcmc = MCMC(nuts_kernel, num_samples=500, warmup_steps=300)
>>> mcmc.run(data)
>>> mcmc.get_samples()['beta'].mean(0)  # doctest: +SKIP
tensor([ 0.9221,  1.9464,  2.9228])
```

sample(*params*)

3.10.5 BlockMassMatrix

class BlockMassMatrix(*init_scale=1.0*)

Bases: `object`

EXPERIMENTAL This class is used to adapt (inverse) mass matrix and provide useful methods to calculate algebraic terms which involves the mass matrix.

The mass matrix will have block structure, which can be specified by using the method *configure()* with the corresponding structured *mass_matrix_shape* arg.

Parameters **init_scale** (*float*) – initial scale to construct the initial mass matrix.

configure(*mass_matrix_shape*, *adapt_mass_matrix=True*, *options={}*)
Sets up an initial mass matrix.

Parameters

- **mass_matrix_shape** (*dict*) – a dict that maps tuples of site names to the shape of the corresponding mass matrix. Each tuple of site names corresponds to a block.
- **adapt_mass_matrix** (*bool*) – a flag to decide whether an adaptation scheme will be used.
- **options** (*dict*) – tensor options to construct the initial mass matrix.

end_adaptation()
Updates the current mass matrix using the adaptation scheme.

inverse_mass_matrix

kinetic_grad(*r*)
Computes the gradient of kinetic energy w.r.t. the momentum *r*. It is equivalent to compute velocity given the momentum *r*.

Parameters **r** (*dict*) – a dictionary maps site names to a tensor momentum.

Returns a dictionary maps site names to the corresponding gradient

mass_matrix_size
A dict that maps site names to the size of the corresponding mass matrix.

scale(*r_unscaled*, *r_prototype*)
Computes *M^{1/2} @ r_unscaled*.

Note that *r* is generated from a gaussian with scale *mass_matrix_sqrt*. This method will scale it.

Parameters

- **r_unscaled** (*dict*) – a dictionary maps site names to a tensor momentum.
- **r_prototype** (*dict*) – a dictionary mapes site names to prototype momentum. Those prototype values are used to get shapes of the scaled version.

Returns a dictionary maps site names to the corresponding tensor

unscale(*r*)
Computes *inv(M^{1/2}) @ r*.

Note that *r* is generated from a gaussian with scale *mass_matrix_sqrt*. This method will unscale it.

Parameters **r** (*dict*) – a dictionary maps site names to a tensor momentum.

Returns a dictionary maps site names to the corresponding tensor

update(*z*, *z_grad*)
Updates the adaptation scheme using the new sample *z* or its grad *z_grad*.

Parameters

- **z** (*dict*) – the current value.
- **z_grad** (*dict*) – grad of the current value.

3.10.6 Utilities

initialize_model(*model*, *model_args=()*, *model_kwargs={}*, *transforms=None*, *max_plate_nesting=None*, *jit_compile=False*, *jit_options=None*, *skip_jit_warnings=False*, *num_chains=1*, *init_strategy=<function init_to_uniform>*, *initial_params=None*)

Given a Python callable with Pyro primitives, generates the following model-specific properties needed for inference using HMC/NUTS kernels:

- initial parameters to be sampled using a HMC kernel,
- a potential function whose input is a dict of parameters in unconstrained space,
- transforms to transform latent sites of *model* to unconstrained space,
- a prototype trace to be used in MCMC to consume traces from sampled parameters.

Parameters

- **model** – a Pyro model which contains Pyro primitives.
- **model_args** (*tuple*) – optional args taken by *model*.
- **model_kwargs** (*dict*) – optional kwargs taken by *model*.
- **transforms** (*dict*) – Optional dictionary that specifies a transform for a sample site with constrained support to unconstrained space. The transform should be invertible, and implement *log_abs_det_jacobian*. If not specified and the model has sites with constrained support, automatic transformations will be applied, as specified in `torch.distributions.constraint_registry`.
- **max_plate_nesting** (*int*) – Optional bound on max number of nested `pyro.plate()` contexts. This is required if model contains discrete sample sites that can be enumerated over in parallel.
- **jit_compile** (*bool*) – Optional parameter denoting whether to use the PyTorch JIT to trace the log density computation, and use this optimized executable trace in the integrator.
- **jit_options** (*dict*) – A dictionary contains optional arguments for `torch.jit.trace()` function.
- **ignore_jit_warnings** (*bool*) – Flag to ignore warnings from the JIT tracer when `jit_compile=True`. Default is False.
- **num_chains** (*int*) – Number of parallel chains. If *num_chains* > *1*, the returned *initial_params* will be a list with *num_chains* elements.
- **init_strategy** (*callable*) – A per-site initialization function. See *Initialization* section for available functions.
- **initial_params** (*dict*) – dict containing initial tensors in unconstrained space to initiate the markov chain.

Returns a tuple of (*initial_params*, *potential_fn*, *transforms*, *prototype_trace*)

diagnostics(*samples*, *group_by_chain=True*)

Gets diagnostics statistics such as effective sample size and split Gelman-Rubin using the samples drawn from the posterior distribution.

Parameters

- **samples** (*dict*) – dictionary of samples keyed by site name.

- **group_by_chain** (*bool*) – If True, each variable in *samples* will be treated as having shape *num_chains x num_samples x sample_shape*. Otherwise, the corresponding shape will be *num_samples x sample_shape* (i.e. without chain dimension).

Returns dictionary of diagnostic stats for each sample site.

3.11 Automatic Guide Generation

3.11.1 AutoGuide

class AutoGuide(*model*, *, *create_plates=None*)

Bases: *pyro.nn.module.PyroModule*

Base class for automatic guides.

Derived classes must implement the `forward()` method, with the same `*args, **kwargs` as the base `model`.

Auto guides can be used individually or combined in an *AutoGuideList* object.

Parameters

- **model** (*callable*) – A pyro model.
- **create_plates** (*callable*) – An optional function inputing the same `*args, **kwargs` as `model()` and returning a `pyro.plate` or iterable of plates. Plates not returned will be created automatically as usual. This is useful for data subsampling.

call(**args*, ***kwargs*)

Method that calls `forward()` and returns parameter values of the guide as a *tuple* instead of a *dict*, which is a requirement for JIT tracing. Unlike `forward()`, this method can be traced by `torch.jit.trace_module()`.

> **Warning:** This method may be removed once PyTorch JIT tracer starts accepting *dict* as valid return types. See *issue <https://github.com/pytorch/pytorch/issues/27743>_*.

median(**args*, ***kwargs*)

Returns the posterior median value of each latent variable.

Returns A dict mapping sample site name to median tensor.

Return type dict

model

sample_latent(***kwargs*)

Samples an encoded latent given the same `*args, **kwargs` as the base `model`.

3.11.2 AutoGuideList

class AutoGuideList(*model*, *, *create_plates=None*)

Bases: `pyro.infer.autoguide.guides.AutoGuide`, `torch.nn.modules.container.ModuleList`

Container class to combine multiple automatic guides.

Example usage:

```
guide = AutoGuideList(my_model)
guide.append(AutoDiagonalNormal(poutine.block(model, hide=["assignment"])))
guide.append(AutoDiscreteParallel(poutine.block(model, expose=["assignment"])))
svi = SVI(model, guide, optim, Trace_ELBO())
```

Parameters **model** (*callable*) – a Pyro model

add(*part*)
Deprecated alias for *append()*.

append(*part*)
Add an automatic guide for part of the model. The guide should have been created by blocking the model to restrict to a subset of sample sites. No two parts should operate on any one sample site.

Parameters **part** (*AutoGuide or callable*) – a partial guide to add

forward(**args*, ***kwargs*)
A composite guide with the same `*args, **kwargs` as the base `model`.

Note: This method is used internally by `Module`. Users should instead use `__call__()`.

Returns A dict mapping sample site name to sampled value.

Return type dict

median(**args*, ***kwargs*)
Returns the posterior median value of each latent variable.

Returns A dict mapping sample site name to median tensor.

Return type dict

3.11.3 AutoCallable

class AutoCallable(*model*, *guide*, *median=<function AutoCallable.<lambda>>*)
Bases: `pyro.infer.autoguide.guides.AutoGuide`

AutoGuide wrapper for simple callable guides.

This is used internally for composing autoguides with custom user-defined guides that are simple callables, e.g.:

```
def my_local_guide(*args, **kwargs):
    ...

guide = AutoGuideList(model)
guide.add(AutoDelta(poutine.block(model, expose=['my_global_param'])))
guide.add(my_local_guide)  # automatically wrapped in an AutoCallable
```

To specify a median callable, you can instead:

```
def my_local_median(*args, **kwargs)
    ...

guide.add(AutoCallable(model, my_local_guide, my_local_median))
```

For more complex guides that need e.g. access to plates, users should instead subclass `AutoGuide`.

Parameters

- **model** (*callable*) – a Pyro model
- **guide** (*callable*) – a Pyro guide (typically over only part of the model)
- **median** (*callable*) – an optional callable returning a dict mapping sample site name to computed median tensor.

forward(**args*, ***kwargs*)

3.11.4 AutoNormal

class AutoNormal(*model*, ***, *init_loc_fn=<function init_to_feasible>*, *init_scale=0.1*, *create_plates=None*)

Bases: pyro.infer.autoguide.guides.AutoGuide

This implementation of *AutoGuide* uses a Normal distribution with a diagonal covariance matrix to construct a guide over the entire latent space. The guide does not depend on the model's `*args, **kwargs`.

It should be equivalent to :class: *AutoDiagonalNormal* , but with more convenient site names and with better support for *TraceMeanField_ELBO* .

In *AutoDiagonalNormal* , if your model has N named parameters with dimensions k_i and sum k_i = D, you get a single vector of length D for your mean, and a single vector of length D for sigmas. This guide gives you N distinct normals that you can call by name.

Usage:

```
guide = AutoNormal(model)
svi = SVI(model, guide, ...)
```

Parameters

- **model** (*callable*) – A Pyro model.
- **init_loc_fn** (*callable*) – A per-site initialization function. See *Initialization* section for available functions.
- **init_scale** (*float*) – Initial scale for the standard deviation of each (unconstrained transformed) latent variable.
- **create_plates** (*callable*) – An optional function inputing the same `*args, **kwargs` as `model()` and returning a `pyro.plate` or iterable of plates. Plates not returned will be created automatically as usual. This is useful for data subsampling.

forward(**args*, ***kwargs*)

An automatic guide with the same `*args, **kwargs` as the base `model`.

Note: This method is used internally by `Module`. Users should instead use `__call__()`.

Returns A dict mapping sample site name to sampled value.

Return type dict

median(**args*, ***kwargs*)

Returns the posterior median value of each latent variable.

Returns A dict mapping sample site name to median tensor.

Return type dict

quantiles(*quantiles*, **args*, ***kwargs*)

Returns posterior quantiles each latent variable. Example:

```
print(guide.quantiles([0.05, 0.5, 0.95]))
```

Parameters **quantiles** (*torch.Tensor or list*) – A list of requested quantiles between 0 and 1.

Returns A dict mapping sample site name to a list of quantile values.

Return type dict

3.11.5 AutoDelta

class AutoDelta(*model*, *init_loc_fn=<function init_to_median>*, ***, *create_plates=None*)

Bases: pyro.infer.autoguide.guides.AutoGuide

This implementation of *AutoGuide* uses Delta distributions to construct a MAP guide over the entire latent space. The guide does not depend on the model's `*args, **kwargs`.

Note: This class does MAP inference in constrained space.

Usage:

```
guide = AutoDelta(model)
svi = SVI(model, guide, ...)
```

Latent variables are initialized using `init_loc_fn()`. To change the default behavior, create a custom `init_loc_fn()` as described in *Initialization* , for example:

```
def my_init_fn(site):
    if site["name"] == "level":
        return torch.tensor([-1., 0., 1.])
    if site["name"] == "concentration":
        return torch.ones(k)
    return init_to_sample(site)
```

Parameters

- **model** (*callable*) – A Pyro model.
- **init_loc_fn** (*callable*) – A per-site initialization function. See *Initialization* section for available functions.
- **create_plates** (*callable*) – An optional function inputing the same `*args, **kwargs` as `model()` and returning a `pyro.plate` or iterable of plates. Plates not returned will be created automatically as usual. This is useful for data subsampling.

forward(**args*, ***kwargs*)

An automatic guide with the same `*args, **kwargs` as the base `model`.

Note: This method is used internally by `Module`. Users should instead use `__call__()`.

Returns A dict mapping sample site name to sampled value.

Return type dict

median(**args*, ***kwargs*)
Returns the posterior median value of each latent variable.

Returns A dict mapping sample site name to median tensor.

Return type dict

3.11.6 AutoContinuous

class AutoContinuous(*model*, *init_loc_fn=<function init_to_median>*)
Bases: pyro.infer.autoguide.guides.AutoGuide

Base class for implementations of continuous-valued Automatic Differentiation Variational Inference [1].

This uses torch.distributions.transforms to transform each constrained latent variable to an unconstrained space, then concatenate all variables into a single unconstrained latent variable. Each derived class implements a *get_posterior()* method returning a distribution over this single unconstrained latent variable.

Assumes model structure and latent dimension are fixed, and all latent variables are continuous.

Parameters **model** (*callable*) – a Pyro model

Reference:

[1] ***Automatic Differentiation Variational Inference*,** Alp Kucukelbir, Dustin Tran, Rajesh Ranganath, Andrew Gelman, David M. Blei

Parameters

- **model** (*callable*) – A Pyro model.
- **init_loc_fn** (*callable*) – A per-site initialization function. See *Initialization* section for available functions.

forward(**args*, ***kwargs*)
An automatic guide with the same `*args, **kwargs` as the base `model`.

Note: This method is used internally by Module. Users should instead use `__call__()`.

Returns A dict mapping sample site name to sampled value.

Return type dict

get_base_dist()
Returns the base distribution of the posterior when reparameterized as a *TransformedDistribution*. This should not depend on the model's **args, **kwargs*.

```
posterior = TransformedDistribution(self.get_base_dist(), self.get_
↪transform(*args, **kwargs))
```

Returns *TorchDistribution* instance representing the base distribution.

get_posterior(**args*, ***kwargs*)
Returns the posterior distribution.

get_transform(**args*, ***kwargs*)
Returns the transform applied to the base distribution when the posterior is reparameterized as a *TransformedDistribution*. This may depend on the model's **args, **kwargs*.

```
posterior = TransformedDistribution(self.get_base_dist(), self.get_
↪transform(*args, **kwargs))
```

Returns a `Transform` instance.

median(**args*, ***kwargs*)
Returns the posterior median value of each latent variable.

Returns A dict mapping sample site name to median tensor.

Return type dict

quantiles(*quantiles*, **args*, ***kwargs*)
Returns posterior quantiles each latent variable. Example:

```
print(guide.quantiles([0.05, 0.5, 0.95]))
```

Parameters **quantiles** (*torch.Tensor or list*) – A list of requested quantiles between 0 and 1.

Returns A dict mapping sample site name to a list of quantile values.

Return type dict

sample_latent(**args*, ***kwargs*)
Samples an encoded latent given the same `*args, **kwargs` as the base `model`.

3.11.7 AutoMultivariateNormal

class AutoMultivariateNormal(*model*, *init_loc_fn=<function init_to_median>*, *init_scale=0.1*)
Bases: `pyro.infer.autoguide.guides.AutoContinuous`

This implementation of *AutoContinuous* uses a Cholesky factorization of a Multivariate Normal distribution to construct a guide over the entire latent space. The guide does not depend on the model's `*args, **kwargs`.

Usage:

```
guide = AutoMultivariateNormal(model)
svi = SVI(model, guide, ...)
```

By default the mean vector is initialized by `init_loc_fn()` and the Cholesky factor is initialized to the identity times a small factor.

Parameters

- **model** (*callable*) – A generative model.
- **init_loc_fn** (*callable*) – A per-site initialization function. See *Initialization* section for available functions.

- **init_scale** (*float*) – Initial scale for the standard deviation of each (unconstrained transformed) latent variable.

get_base_dist()

get_posterior(**args*, ***kwargs*)
Returns a MultivariateNormal posterior distribution.

get_transform(**args*, ***kwargs*)

3.11.8 AutoDiagonalNormal

class AutoDiagonalNormal(*model*, *init_loc_fn=<function init_to_median>*, *init_scale=0.1*)
Bases: pyro.infer.autoguide.guides.AutoContinuous

This implementation of *AutoContinuous* uses a Normal distribution with a diagonal covariance matrix to construct a guide over the entire latent space. The guide does not depend on the model's `*args, **kwargs`.

Usage:

```
guide = AutoDiagonalNormal(model)
svi = SVI(model, guide, ...)
```

By default the mean vector is initialized to zero and the scale is initialized to the identity times a small factor.

Parameters

- **model** (*callable*) – A generative model.
- **init_loc_fn** (*callable*) – A per-site initialization function. See *Initialization* section for available functions.
- **init_scale** (*float*) – Initial scale for the standard deviation of each (unconstrained transformed) latent variable.

get_base_dist()

get_posterior(**args*, ***kwargs*)
Returns a diagonal Normal posterior distribution.

get_transform(**args*, ***kwargs*)

3.11.9 AutoLowRankMultivariateNormal

class AutoLowRankMultivariateNormal(*model*, *init_loc_fn=<function init_to_median>*, *init_scale=0.1*, *rank=None*)
Bases: pyro.infer.autoguide.guides.AutoContinuous

This implementation of *AutoContinuous* uses a low rank plus diagonal Multivariate Normal distribution to construct a guide over the entire latent space. The guide does not depend on the model's `*args, **kwargs`.

Usage:

```
guide = AutoLowRankMultivariateNormal(model, rank=10)
svi = SVI(model, guide, ...)
```

By default the `cov_diag` is initialized to a small constant and the `cov_factor` is initialized randomly such that on average `cov_factor.matmul(cov_factor.t())` has the same scale as `cov_diag`.

Parameters

- **model** (*callable*) – A generative model.
- **rank** (*int or None*) – The rank of the low-rank part of the covariance matrix. Defaults to approximately `sqrt(latent dim)`.
- **init_loc_fn** (*callable*) – A per-site initialization function. See *Initialization* section for available functions.
- **init_scale** (*float*) – Approximate initial scale for the standard deviation of each (unconstrained transformed) latent variable.

get_posterior(**args*, ***kwargs*)
Returns a LowRankMultivariateNormal posterior distribution.

3.11.10 AutoNormalizingFlow

class AutoNormalizingFlow(*model*, *init_transform_fn*)
Bases: `pyro.infer.autoguide.guides.AutoContinuous`

This implementation of *AutoContinuous* uses a Diagonal Normal distribution transformed via a sequence of bijective transforms (e.g. various *TransformModule* subclasses) to construct a guide over the entire latent space. The guide does not depend on the model's `*args, **kwargs`.

Usage:

```
transform_init = partial(iterated, block_autoregressive,
                         repeats=2)
guide = AutoNormalizingFlow(model, transform_init)
svi = SVI(model, guide, ...)
```

Parameters

- **model** (*callable*) – a generative model
- **init_transform_fn** – a callable which when provided with the latent dimension returns an instance of `Transform`, or *TransformModule* if the transform has trainable params.

get_base_dist()

get_posterior(**args*, ***kwargs*)

get_transform(**args*, ***kwargs*)

3.11.11 AutoIAFNormal

class AutoIAFNormal(*model*, *hidden_dim=None*, *init_loc_fn=None*, *num_transforms=1*, ***init_transform_kwargs*)
Bases: `pyro.infer.autoguide.guides.AutoNormalizingFlow`

This implementation of *AutoContinuous* uses a Diagonal Normal distribution transformed via a *AffineAutoregressive* to construct a guide over the entire latent space. The guide does not depend on the model's `*args, **kwargs`.

Usage:

```
guide = AutoIAFNormal(model, hidden_dim=latent_dim)
svi = SVI(model, guide, ...)
```

Parameters

- **model** (*callable*) – a generative model
- **hidden_dim** (*list[int]*) – number of hidden dimensions in the IAF
- **init_loc_fn** (*callable*) – A per-site initialization function. See *Initialization* section for available functions.

  Warning: This argument is only to preserve backwards compatibility and has no effect in practice.

- **num_transforms** (*int*) – number of *AffineAutoregressive* transforms to use in sequence.
- **init_transform_kwargs** – other keyword arguments taken by *affine_autoregressive()*.

3.11.12 AutoLaplaceApproximation

class AutoLaplaceApproximation(*model*, *init_loc_fn=<function init_to_median>*)

Bases: pyro.infer.autoguide.guides.AutoContinuous

Laplace approximation (quadratic approximation) approximates the posterior $\log p(z|x)$ by a multivariate normal distribution in the unconstrained space. Under the hood, it uses Delta distributions to construct a MAP guide over the entire (unconstrained) latent space. Its covariance is given by the inverse of the hessian of $-\log p(x, z)$ at the MAP point of z.

Usage:

```
delta_guide = AutoLaplaceApproximation(model)
svi = SVI(model, delta_guide, ...)
# ...then train the delta_guide...
guide = delta_guide.laplace_approximation()
```

By default the mean vector is initialized to an empirical prior median.

Parameters

- **model** (*callable*) – a generative model
- **init_loc_fn** (*callable*) – A per-site initialization function. See *Initialization* section for available functions.

get_posterior(**args*, ***kwargs*)

Returns a Delta posterior distribution for MAP inference.

laplace_approximation(**args*, ***kwargs*)

Returns a *AutoMultivariateNormal* instance whose posterior's *loc* and *scale_tril* are given by Laplace approximation.

3.11.13 AutoDiscreteParallel

class AutoDiscreteParallel(*model*, ***, *create_plates=None*)

Bases: pyro.infer.autoguide.guides.AutoGuide

A discrete mean-field guide that learns a latent discrete distribution for each discrete site in the model.

forward(**args*, ***kwargs*)
An automatic guide with the same `*args, **kwargs` as the base `model`.

Note: This method is used internally by `Module`. Users should instead use `__call__()`.

Returns A dict mapping sample site name to sampled value.

Return type dict

3.11.14 Initialization

The pyro.infer.autoguide.initialization module contains initialization functions for automatic guides.

The standard interface for initialization is a function that inputs a Pyro trace `site` dict and returns an appropriately sized `value` to serve as an initial constrained value for a guide estimate.

init_to_feasible(*site=None*)
Initialize to an arbitrary feasible point, ignoring distribution parameters.

init_to_sample(*site=None*)
Initialize to a random sample from the prior.

init_to_median(*site=None*, *num_samples=15*)
Initialize to the prior median; fallback to a feasible point if median is undefined.

init_to_mean(*site=None*)
Initialize to the prior mean; fallback to median if mean is undefined.

init_to_uniform(*site=None*, *radius=2*)
Initialize to a random point in the area `(-radius, radius)` of unconstrained domain.

Parameters **radius** (*float*) – specifies the range to draw an initial point in the unconstrained domain.

init_to_value(*site=None*, *values={}*)
Initialize to the value specified in `values`. We defer to *init_to_uniform()* strategy for sites which do not appear in `values`.

Parameters **values** (*dict*) – dictionary of initial values keyed by site name.

init_to_generated(*site=None*, *generate=<function <lambda>>*)
Initialize to another initialization strategy returned by the callback `generate` which is called once per model execution.

This is like *init_to_value()* but can produce different (e.g. random) values once per model execution. For example to generate values and return `init_to_value` you could define:

```
def generate():
    values = {"x": torch.randn(100), "y": torch.rand(5)}
    return init_to_value(values=values)

my_init_fn = init_to_generated(generate=generate)
```

Parameters **generate** (*callable*) – A callable returning another initialization function, e.g. returning an `init_to_value(values={...})` populated with a dictionary of random samples.

class InitMessenger(*init_fn*)
Bases: *pyro.poutine.messenger.Messenger*

Initializes a site by replacing `.sample()` calls with values drawn from an initialization strategy. This is mainly for internal use by autoguide classes.

Parameters **init_fn** (*callable*) – An initialization function.

3.12 Reparameterizers

The *pyro.infer.reparam* module contains reparameterization strategies for the *pyro.poutine.handlers.reparam()* effect. These are useful for altering geometry of a poorly-conditioned parameter space to make the posterior better shaped. These can be used with a variety of inference algorithms, e.g. `Auto*Normal` guides and MCMC.

class Reparam
Base class for reparameterizers.

__call__(*name*, *fn*, *obs*)

Parameters

- **name** (*str*) – A sample site name.
- **fn** (`TorchDistribution`) – A distribution.
- **obs** (*Tensor*) – Observed value or None.

Returns A pair (`new_fn`, `value`).

3.12.1 Conjugate Updating

class ConjugateReparam(*guide*)
Bases: *pyro.infer.reparam.reparam.Reparam*

EXPERIMENTAL Reparameterize to a conjugate updated distribution.

This updates a prior distribution `fn` using the *conjugate_update()* method. The guide may be either a distribution object or a callable inputting model `*args,**kwargs` and returning a distribution object. The guide may be approximate or learned.

For example consider the model and naive variational guide:

```
total = torch.tensor(10.)
count = torch.tensor(2.)

def model():
    prob = pyro.sample("prob", dist.Beta(0.5, 1.5))
    pyro.sample("count", dist.Binomial(total, prob), obs=count)

guide = AutoDiagonalNormal(model)  # learns the posterior over prob
```

Instead of using this learned guide, we can hand-compute the conjugate posterior distribution over "prob", and then use a simpler guide during inference, in this case an empty guide:

```
reparam_model = poutine.reparam(model, {
    "prob": ConjugateReparam(dist.Beta(1 + count, 1 + total - count))
})
```

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```
def reparam_guide():
    pass  # nothing remains to be modeled!
```

Parameters **guide** (*Distribution or callable*) – A likelihood distribution or a callable returning a guide distribution. Only a few distributions are supported, depending on the prior distribution's *conjugate_update()* implementation.

__call__(*name*, *fn*, *obs*)

3.12.2 Loc-Scale Decentering

class LocScaleReparam(*centered=None*, *shape_params=()*)

Bases: *pyro.infer.reparam.reparam.Reparam*

Generic decentering reparameterizer [1] for latent variables parameterized by `loc` and `scale` (and possibly additional `shape_params`).

This reparameterization works only for latent variables, not likelihoods.

[1] Maria I. Gorinova, Dave Moore, Matthew D. Hoffman (2019) "Automatic Reparameterisation of Probabilistic Programs" https://arxiv.org/pdf/1906.03028.pdf

Parameters

- **centered** (*float*) – optional centered parameter. If None (default) learn a per-site per-element centering parameter in `[0,1]`. If 0, fully decenter the distribution; if 1, preserve the centered distribution unchanged.
- **shape_params** (*tuple or list*) – list of additional parameter names to copy unchanged from the centered to decentered distribution.

__call__(*name*, *fn*, *obs*)

3.12.3 Gumbel-Softmax

class GumbelSoftmaxReparam

Bases: *pyro.infer.reparam.reparam.Reparam*

Reparametrizer for *RelaxedOneHotCategorical* latent variables.

This is useful for transforming multimodal posteriors to unimodal posteriors. Note this increases the latent dimension by 1 per event.

This reparameterization works only for latent variables, not likelihoods.

__call__(*name*, *fn*, *obs*)

3.12.4 Transformed Distributions

class TransformReparam

Bases: *pyro.infer.reparam.reparam.Reparam*

Reparameterizer for `pyro.distributions.torch.TransformedDistribution` latent variables.

This is useful for transformed distributions with complex, geometry-changing transforms, where the posterior has simple shape in the space of `base_dist`.

This reparameterization works only for latent variables, not likelihoods.

__call__(*name*, *fn*, *obs*)

3.12.5 Discrete Cosine Transform

class DiscreteCosineReparam(*dim=-1*, *smooth=0.0*, *, *experimental_allow_batch=False*)
Bases: *pyro.infer.reparam.unit_jacobian.UnitJacobianReparam*

Discrete Cosine reparameterizer, using a *DiscreteCosineTransform*.

This is useful for sequential models where coupling along a time-like axis (e.g. a banded precision matrix) introduces long-range correlation. This reparameterizes to a frequency-domain representation where posterior covariance should be closer to diagonal, thereby improving the accuracy of diagonal guides in SVI and improving the effectiveness of a diagonal mass matrix in HMC.

When reparameterizing variables that are approximately continuous along the time dimension, set `smooth=1`. For variables that are approximately continuously differentiable along the time axis, set `smooth=2`.

This reparameterization works only for latent variables, not likelihoods.

Parameters

- **dim** (*int*) – Dimension along which to transform. Must be negative. This is an absolute dim counting from the right.
- **smooth** (*float*) – Smoothing parameter. When 0, this transforms white noise to white noise; when 1 this transforms Brownian noise to to white noise; when -1 this transforms violet noise to white noise; etc. Any real number is allowed. https://en.wikipedia.org/wiki/Colors_of_noise.

3.12.6 Haar Transform

class HaarReparam(*dim=-1*, *flip=False*, *, *experimental_allow_batch=False*)
Bases: *pyro.infer.reparam.unit_jacobian.UnitJacobianReparam*

Haar wavelet reparameterizer, using a *HaarTransform*.

This is useful for sequential models where coupling along a time-like axis (e.g. a banded precision matrix) introduces long-range correlation. This reparameterizes to a frequency-domain representation where posterior covariance should be closer to diagonal, thereby improving the accuracy of diagonal guides in SVI and improving the effectiveness of a diagonal mass matrix in HMC.

This reparameterization works only for latent variables, not likelihoods.

Parameters

- **dim** (*int*) – Dimension along which to transform. Must be negative. This is an absolute dim counting from the right.
- **flip** (*bool*) – Whether to flip the time axis before applying the Haar transform. Defaults to false.

3.12.7 Unit Jacobian Transforms

class UnitJacobianReparam(*transform*, *suffix='transformed'*, ***, *experimental_allow_batch=False*)
Bases: *pyro.infer.reparam.reparam.Reparam*

Reparameterizer for `Transform` objects whose Jacobian determinant is one.

Parameters

- **transform** (*Transform*) – A transform whose Jacobian has determinant 1.
- **suffix** (*str*) – A suffix to append to the transformed site.

__call__(*name*, *fn*, *obs*)

3.12.8 StudentT Distributions

class StudentTReparam
Bases: *pyro.infer.reparam.reparam.Reparam*

Auxiliary variable reparameterizer for *StudentT* random variables.

This is useful in combination with *LinearHMMReparam* because it allows StudentT processes to be treated as conditionally Gaussian processes, permitting cheap inference via *GaussianHMM* .

This reparameterizes a *StudentT* by introducing an auxiliary *Gamma* variable conditioned on which the result is *Normal* .

__call__(*name*, *fn*, *obs*)

3.12.9 Stable Distributions

class LatentStableReparam
Bases: *pyro.infer.reparam.reparam.Reparam*

Auxiliary variable reparameterizer for *Stable* latent variables.

This is useful in inference of latent *Stable* variables because the *log_prob()* is not implemented.

This uses the Chambers-Mallows-Stuck method [1], creating a pair of parameter-free auxiliary distributions (`Uniform(-pi/2,pi/2)` and `Exponential(1)`) with well-defined `.log_prob()` methods, thereby permitting use of reparameterized stable distributions in likelihood-based inference algorithms like SVI and MCMC.

This reparameterization works only for latent variables, not likelihoods. For likelihood-compatible reparameterization see *SymmetricStableReparam* or *StableReparam* .

[1] J.P. Nolan (2017). Stable Distributions: Models for Heavy Tailed Data. http://fs2.american.edu/jpnolan/www/stable/chap1.pdf

__call__(*name*, *fn*, *obs*)

class SymmetricStableReparam
Bases: *pyro.infer.reparam.reparam.Reparam*

Auxiliary variable reparameterizer for symmetric *Stable* random variables (i.e. those for which `skew=0`).

This is useful in inference of symmetric *Stable* variables because the *log_prob()* is not implemented.

This reparameterizes a symmetric *Stable* random variable as a totally-skewed (`skew=1`) *Stable* scale mixture of *Normal* random variables. See Proposition 3. of [1] (but note we differ since `Stable` uses Nolan's continuous S0 parameterization).

[1] Alvaro Cartea and Sam Howison (2009) "Option Pricing with Levy-Stable Processes" https://pdfs.semanticscholar.org/4d66/c91b136b2a38117dd16c2693679f5341c616.pdf

__call__(*name*, *fn*, *obs*)

class StableReparam

Bases: *pyro.infer.reparam.reparam.Reparam*

Auxiliary variable reparameterizer for arbitrary *Stable* random variables.

This is useful in inference of non-symmetric *Stable* variables because the *log_prob()* is not implemented.

This reparameterizes a *Stable* random variable as sum of two other stable random variables, one symmetric and the other totally skewed (applying Property 2.3.a of [1]). The totally skewed variable is sampled as in *LatentStableReparam*, and the symmetric variable is decomposed as in *SymmetricStableReparam*.

[1] V. M. Zolotarev (1986) "One-dimensional stable distributions"

__call__(*name*, *fn*, *obs*)

3.12.10 Hidden Markov Models

class LinearHMMReparam(*init=None*, *trans=None*, *obs=None*)

Bases: *pyro.infer.reparam.reparam.Reparam*

Auxiliary variable reparameterizer for *LinearHMM* random variables.

This defers to component reparameterizers to create auxiliary random variables conditioned on which the process becomes a *GaussianHMM*. If the `observation_dist` is a *TransformedDistribution* this reorders those transforms so that the result is a *TransformedDistribution* of *GaussianHMM*.

This is useful for training the parameters of a *LinearHMM* distribution, whose *log_prob()* method is undefined. To perform inference in the presence of non-Gaussian factors such as *Stable()*, *StudentT()* or *LogNormal()*, configure with *StudentTReparam*, *StableReparam*, *SymmetricStableReparam*, etc. component reparameterizers for `init`, `trans`, and `scale`. For example:

```
hmm = LinearHMM(
    init_dist=Stable(1,0,1,0).expand([2]).to_event(1),
    trans_matrix=torch.eye(2),
    trans_dist=MultivariateNormal(torch.zeros(2), torch.eye(2)),
    obs_matrix=torch.eye(2),
    obs_dist=TransformedDistribution(
        Stable(1.5,-0.5,1.0).expand([2]).to_event(1),
        ExpTransform()))

rep = LinearHMMReparam(init=SymmetricStableReparam(),
                       obs=StableReparam())

with poutine.reparam(config={"hmm": rep}):
    pyro.sample("hmm", hmm, obs=data)
```

Parameters

- **init** (Reparam) – Optional reparameterizer for the initial distribution.
- **trans** (Reparam) – Optional reparameterizer for the transition distribution.
- **obs** (Reparam) – Optional reparameterizer for the observation distribution.

__call__(*name*, *fn*, *obs*)

3.12.11 Site Splitting

class SplitReparam(*sections*, *dim*)
Bases: *pyro.infer.reparam.reparam.Reparam*

Reparameterizer to split a random variable along a dimension, similar to `torch.split()`.

This is useful for treating different parts of a tensor with different reparameterizers or inference methods. For example when performing HMC inference on a time series, you can first apply *DiscreteCosineReparam* or *HaarReparam*, then apply *SplitReparam* to split into low-frequency and high-frequency components, and finally add the low-frequency components to the `full_mass` matrix together with globals.

Parameters

- **sections** – Size of a single chunk or list of sizes for each chunk.
- **dim** (*int*) – Dimension along which to split. Defaults to -1.

Type list(int)

__call__(*name*, *fn*, *obs*)

3.12.12 Neural Transport

class NeuTraReparam(*guide*)
Bases: *pyro.infer.reparam.reparam.Reparam*

Neural Transport reparameterizer [1] of multiple latent variables.

This uses a trained *AutoContinuous* guide to alter the geometry of a model, typically for use e.g. in MCMC. Example usage:

```
# Step 1. Train a guide
guide = AutoIAFNormal(model)
svi = SVI(model, guide, ...)
# ...train the guide...

# Step 2. Use trained guide in NeuTra MCMC
neutra = NeuTraReparam(guide)
model = poutine.reparam(model, config=lambda _: neutra)
nuts = NUTS(model)
# ...now use the model in HMC or NUTS...
```

This reparameterization works only for latent variables, not likelihoods. Note that all sites must share a single common *NeuTraReparam* instance, and that the model must have static structure.

[1] Hoffman, M. et al. (2019) "NeuTra-lizing Bad Geometry in Hamiltonian Monte Carlo Using Neural Transport" https://arxiv.org/abs/1903.03704

Parameters **guide** (`AutoContinuous`) – A trained guide.

reparam(*fn=None*)

__call__(*name*, *fn*, *obs*)

transform_sample(*latent*)

Given latent samples from the warped posterior (with a possible batch dimension), return a *dict* of samples from the latent sites in the model.

Parameters **latent** – sample from the warped posterior (possibly batched). Note that the batch dimension must not collide with plate dimensions in the model, i.e. any batch dims *d* < - *max_plate_nesting*.

Returns a *dict* of samples keyed by latent sites in the model.

Return type dict

CHAPTER 4

Distributions

4.1 PyTorch Distributions

Most distributions in Pyro are thin wrappers around PyTorch distributions. For details on the PyTorch distribution interface, see `torch.distributions.distribution.Distribution`. For differences between the Pyro and PyTorch interfaces, see *TorchDistributionMixin*.

4.1.1 Bernoulli

class Bernoulli(*probs=None*, *logits=None*, *validate_args=None*)
Wraps `torch.distributions.bernoulli.Bernoulli` with *TorchDistributionMixin*.

4.1.2 Beta

class Beta(*concentration1*, *concentration0*, *validate_args=None*)
Wraps `torch.distributions.beta.Beta` with *TorchDistributionMixin*.

4.1.3 Binomial

class Binomial(*total_count=1*, *probs=None*, *logits=None*, *validate_args=None*)
Wraps `torch.distributions.binomial.Binomial` with *TorchDistributionMixin*.

4.1.4 Categorical

class Categorical(*probs=None*, *logits=None*, *validate_args=None*)
Wraps `torch.distributions.categorical.Categorical` with *TorchDistributionMixin*.

4.1.5 Cauchy

class Cauchy(*loc*, *scale*, *validate_args=None*)
Wraps `torch.distributions.cauchy.Cauchy` with *TorchDistributionMixin*.

4.1.6 Chi2

class Chi2(*df*, *validate_args=None*)
Wraps `torch.distributions.chi2.Chi2` with *TorchDistributionMixin*.

4.1.7 ContinuousBernoulli

class ContinuousBernoulli(*probs=None*, *logits=None*, *lims=(0.499, 0.501)*, *validate_args=None*)
Wraps `torch.distributions.continuous_bernoulli.ContinuousBernoulli` with *TorchDistributionMixin*.

4.1.8 Dirichlet

class Dirichlet(*concentration*, *validate_args=None*)
Wraps `torch.distributions.dirichlet.Dirichlet` with *TorchDistributionMixin*.

4.1.9 Exponential

class Exponential(*rate*, *validate_args=None*)
Wraps `torch.distributions.exponential.Exponential` with *TorchDistributionMixin*.

4.1.10 ExponentialFamily

class ExponentialFamily(*batch_shape=torch.Size([])*, *event_shape=torch.Size([])*, *validate_args=None*)
Wraps `torch.distributions.exp_family.ExponentialFamily` with *TorchDistributionMixin*.

4.1.11 FisherSnedecor

class FisherSnedecor(*df1*, *df2*, *validate_args=None*)
Wraps `torch.distributions.fishersnedecor.FisherSnedecor` with *TorchDistributionMixin*.

4.1.12 Gamma

class Gamma(*concentration*, *rate*, *validate_args=None*)
Wraps `torch.distributions.gamma.Gamma` with *TorchDistributionMixin*.

4.1.13 Geometric

class Geometric(*probs=None*, *logits=None*, *validate_args=None*)
Wraps `torch.distributions.geometric.Geometric` with *TorchDistributionMixin*.

4.1.14 Gumbel

class Gumbel(*loc*, *scale*, *validate_args=None*)
Wraps `torch.distributions.gumbel.Gumbel` with *TorchDistributionMixin*.

4.1.15 HalfCauchy

class HalfCauchy(*scale*, *validate_args=None*)
Wraps `torch.distributions.half_cauchy.HalfCauchy` with *TorchDistributionMixin*.

4.1.16 HalfNormal

class HalfNormal(*scale*, *validate_args=None*)
Wraps `torch.distributions.half_normal.HalfNormal` with *TorchDistributionMixin*.

4.1.17 Independent

class Independent(*base_distribution*, *reinterpreted_batch_ndims*, *validate_args=None*)
Wraps `torch.distributions.independent.Independent` with *TorchDistributionMixin*.

4.1.18 Laplace

class Laplace(*loc*, *scale*, *validate_args=None*)
Wraps `torch.distributions.laplace.Laplace` with *TorchDistributionMixin*.

4.1.19 LogNormal

class LogNormal(*loc*, *scale*, *validate_args=None*)
Wraps `torch.distributions.log_normal.LogNormal` with *TorchDistributionMixin*.

4.1.20 LogisticNormal

class LogisticNormal(*loc*, *scale*, *validate_args=None*)
Wraps `torch.distributions.logistic_normal.LogisticNormal` with *TorchDistributionMixin*.

4.1.21 LowRankMultivariateNormal

class LowRankMultivariateNormal(*loc*, *cov_factor*, *cov_diag*, *validate_args=None*)
Wraps `torch.distributions.lowrank_multivariate_normal.LowRankMultivariateNormal` with *TorchDistributionMixin*.

4.1.22 MixtureSameFamily

class MixtureSameFamily(*mixture_distribution*, *component_distribution*, *validate_args=None*)
Wraps `torch.distributions.mixture_same_family.MixtureSameFamily` with *TorchDistributionMixin*.

4.1.23 Multinomial

class Multinomial(*total_count=1*, *probs=None*, *logits=None*, *validate_args=None*)
Wraps `torch.distributions.multinomial.Multinomial` with *TorchDistributionMixin*.

4.1.24 MultivariateNormal

class MultivariateNormal(*loc*, *covariance_matrix=None*, *precision_matrix=None*, *scale_tril=None*, *validate_args=None*)
Wraps `torch.distributions.multivariate_normal.MultivariateNormal` with *TorchDistributionMixin*.

4.1.25 NegativeBinomial

class NegativeBinomial(*total_count*, *probs=None*, *logits=None*, *validate_args=None*)
Wraps `torch.distributions.negative_binomial.NegativeBinomial` with *TorchDistributionMixin*.

4.1.26 Normal

class Normal(*loc*, *scale*, *validate_args=None*)
Wraps `torch.distributions.normal.Normal` with *TorchDistributionMixin*.

4.1.27 OneHotCategorical

class OneHotCategorical(*probs=None*, *logits=None*, *validate_args=None*)
Wraps `torch.distributions.one_hot_categorical.OneHotCategorical` with *TorchDistributionMixin*.

4.1.28 Pareto

class Pareto(*scale*, *alpha*, *validate_args=None*)
Wraps `torch.distributions.pareto.Pareto` with *TorchDistributionMixin*.

4.1.29 Poisson

class Poisson(*rate*, *validate_args=None*)
Wraps `torch.distributions.poisson.Poisson` with *TorchDistributionMixin*.

4.1.30 RelaxedBernoulli

class RelaxedBernoulli(*temperature*, *probs=None*, *logits=None*, *validate_args=None*)
Wraps `torch.distributions.relaxed_bernoulli.RelaxedBernoulli` with *TorchDistributionMixin*.

4.1.31 RelaxedOneHotCategorical

class RelaxedOneHotCategorical(*temperature*, *probs=None*, *logits=None*, *validate_args=None*)
Wraps `torch.distributions.relaxed_categorical.RelaxedOneHotCategorical` with *TorchDistributionMixin*.

4.1.32 StudentT

class StudentT(*df*, *loc=0.0*, *scale=1.0*, *validate_args=None*)
Wraps `torch.distributions.studentT.StudentT` with *TorchDistributionMixin*.

4.1.33 TransformedDistribution

class TransformedDistribution(*base_distribution*, *transforms*, *validate_args=None*)
Wraps `torch.distributions.transformed_distribution.TransformedDistribution` with *TorchDistributionMixin*.

4.1.34 Uniform

class Uniform(*low*, *high*, *validate_args=None*)
Wraps `torch.distributions.uniform.Uniform` with *TorchDistributionMixin*.

4.1.35 VonMises

class VonMises(*loc*, *concentration*, *validate_args=None*)
Wraps `torch.distributions.von_mises.VonMises` with *TorchDistributionMixin*.

4.1.36 Weibull

class Weibull(*scale*, *concentration*, *validate_args=None*)
Wraps `torch.distributions.weibull.Weibull` with *TorchDistributionMixin*.

4.2 Pyro Distributions

4.2.1 Abstract Distribution

class Distribution
Bases: `object`

Base class for parameterized probability distributions.

Distributions in Pyro are stochastic function objects with *sample()* and *log_prob()* methods. Distribution are stochastic functions with fixed parameters:

```
d = dist.Bernoulli(param)
x = d()                                 # Draws a random sample.
p = d.log_prob(x)                       # Evaluates log probability of x.
```

Implementing New Distributions:

Derived classes must implement the methods: *sample()*, *log_prob()*.

Examples:

Take a look at the examples to see how they interact with inference algorithms.

has_rsample = False

has_enumerate_support = False

__call__(**args*, ***kwargs*)
Samples a random value (just an alias for `.sample(*args, **kwargs)`).

For tensor distributions, the returned tensor should have the same `.shape` as the parameters.

Returns A random value.

Return type torch.Tensor

sample(**args*, ***kwargs*)
Samples a random value.

For tensor distributions, the returned tensor should have the same `.shape` as the parameters, unless otherwise noted.

Parameters **sample_shape** (*torch.Size*) – the size of the iid batch to be drawn from the distribution.

Returns A random value or batch of random values (if parameters are batched). The shape of the result should be `self.shape()`.

Return type torch.Tensor

log_prob(*x*, **args*, ***kwargs*)
Evaluates log probability densities for each of a batch of samples.

Parameters **x** (*torch.Tensor*) – A single value or a batch of values batched along axis 0.

Returns log probability densities as a one-dimensional `Tensor` with same batch size as value and params. The shape of the result should be `self.batch_size`.

Return type torch.Tensor

score_parts(*x*, **args*, ***kwargs*)
Computes ingredients for stochastic gradient estimators of ELBO.

The default implementation is correct both for non-reparameterized and for fully reparameterized distributions. Partially reparameterized distributions should override this method to compute correct *.score_function* and *.entropy_term* parts.

Setting `.has_rsample` on a distribution instance will determine whether inference engines like *SVI* use reparameterized samplers or the score function estimator.

Parameters **x** (*torch.Tensor*) – A single value or batch of values.

Returns A *ScoreParts* object containing parts of the ELBO estimator.

Return type ScoreParts

enumerate_support(*expand=True*)

Returns a representation of the parametrized distribution's support, along the first dimension. This is implemented only by discrete distributions.

Note that this returns support values of all the batched RVs in lock-step, rather than the full cartesian product.

Parameters **expand** (*bool*) – whether to expand the result to a tensor of shape `(n,) + batch_shape + event_shape`. If false, the return value has unexpanded shape `(n,) + (1,)*len(batch_shape) + event_shape` which can be broadcasted to the full shape.

Returns An iterator over the distribution's discrete support.

Return type iterator

conjugate_update(*other*)

EXPERIMENTAL Creates an updated distribution fusing information from another compatible distribution. This is supported by only a few conjugate distributions.

This should satisfy the equation:

```
fg, log_normalizer = f.conjugate_update(g)
assert f.log_prob(x) + g.log_prob(x) == fg.log_prob(x) + log_normalizer
```

Note this is equivalent to `funsor.ops.add` on `Funsor` distributions, but we return a lazy sum `(updated, log_normalizer)` because PyTorch distributions must be normalized. Thus *`conjugate_update()`* should commute with `dist_to_funsor()` and `tensor_to_funsor()`

```
dist_to_funsor(f) + dist_to_funsor(g)
  == dist_to_funsor(fg) + tensor_to_funsor(log_normalizer)
```

Parameters **other** – A distribution representing `p(data|latent)` but normalized over `latent` rather than `data`. Here `latent` is a candidate sample from `self` and `data` is a ground observation of unrelated type.

Returns a pair `(updated,log_normalizer)` where `updated` is an updated distribution of type `type(self)`, and `log_normalizer` is a `Tensor` representing the normalization factor.

has_rsample_(*value*)

Force reparameterized or detached sampling on a single distribution instance. This sets the `.has_rsample` attribute in-place.

This is useful to instruct inference algorithms to avoid reparameterized gradients for variables that discontinuously determine downstream control flow.

Parameters **value** (*bool*) – Whether samples will be pathwise differentiable.

Returns self

Return type *Distribution*

rv

EXPERIMENTAL Switch to the Random Variable DSL for applying transformations to random variables. Supports either chaining operations or arithmetic operator overloading.

Example usage:

```
# This should be equivalent to an Exponential distribution.
Uniform(0, 1).rv.log().neg().dist

# These two distributions Y1, Y2 should be the same
X = Uniform(0, 1).rv
Y1 = X.mul(4).pow(0.5).sub(1).abs().neg().dist
Y2 = (-abs((4*X)**(0.5) - 1)).dist
```

Returns A :class: *~pyro.contrib.randomvariable.random_variable.RandomVariable* object wrapping this distribution.

Return type *RandomVariable*

4.2.2 TorchDistributionMixin

class TorchDistributionMixin

Bases: pyro.distributions.distribution.Distribution

Mixin to provide Pyro compatibility for PyTorch distributions.

You should instead use *TorchDistribution* for new distribution classes.

This is mainly useful for wrapping existing PyTorch distributions for use in Pyro. Derived classes must first inherit from `torch.distributions.distribution.Distribution` and then inherit from *TorchDistributionMixin*.

__call__(*sample_shape=torch.Size([])*)

Samples a random value.

This is reparameterized whenever possible, calling `rsample()` for reparameterized distributions and `sample()` for non-reparameterized distributions.

Parameters **sample_shape** (*torch.Size*) – the size of the iid batch to be drawn from the distribution.

Returns A random value or batch of random values (if parameters are batched). The shape of the result should be *self.shape()*.

Return type torch.Tensor

event_dim

Returns Number of dimensions of individual events.

Return type int

shape(*sample_shape=torch.Size([])*)

The tensor shape of samples from this distribution.

Samples are of shape:

```
d.shape(sample_shape) == sample_shape + d.batch_shape + d.event_shape
```

Parameters **sample_shape** (*torch.Size*) – the size of the iid batch to be drawn from the distribution.

Returns Tensor shape of samples.

Return type torch.Size

expand(*batch_shape*, *_instance=None*)
Returns a new ExpandedDistribution instance with batch dimensions expanded to *batch_shape*.

Parameters

- **batch_shape** (*tuple*) – batch shape to expand to.
- **_instance** – unused argument for compatibility with torch.distributions.Distribution.expand()

Returns an instance of *ExpandedDistribution*.

Return type ExpandedDistribution

expand_by(*sample_shape*)
Expands a distribution by adding sample_shape to the left side of its batch_shape.

To expand internal dims of self.batch_shape from 1 to something larger, use *expand()* instead.

Parameters **sample_shape** (*torch.Size*) – The size of the iid batch to be drawn from the distribution.

Returns An expanded version of this distribution.

Return type ExpandedDistribution

reshape(*sample_shape=None*, *extra_event_dims=None*)

to_event(*reinterpreted_batch_ndims=None*)
Reinterprets the n rightmost dimensions of this distributions batch_shape as event dims, adding them to the left side of event_shape.

Example:

```
>>> [d1.batch_shape, d1.event_shape]
[torch.Size([2, 3]), torch.Size([4, 5])]
>>> d2 = d1.to_event(1)
>>> [d2.batch_shape, d2.event_shape]
[torch.Size([2]), torch.Size([3, 4, 5])]
>>> d3 = d1.to_event(2)
>>> [d3.batch_shape, d3.event_shape]
[torch.Size([]), torch.Size([2, 3, 4, 5])]
```

Parameters **reinterpreted_batch_ndims** (*int*) – The number of batch dimensions to reinterpret as event dimensions. May be negative to remove dimensions from an pyro.distributions.torch.Independent . If None, convert all dimensions to event dimensions.

Returns A reshaped version of this distribution.

Return type pyro.distributions.torch.Independent

independent(*reinterpreted_batch_ndims=None*)

mask(*mask*)
Masks a distribution by a boolean or boolean-valued tensor that is broadcastable to the distributions batch_shape .

Parameters **mask** (*bool or torch.Tensor*) – A boolean or boolean valued tensor.

Returns A masked copy of this distribution.

Return type MaskedDistribution

4.2.3 TorchDistribution

class TorchDistribution(*batch_shape=torch.Size([])*, *event_shape=torch.Size([])*, *validate_args=None*)

Bases: `torch.distributions.distribution.Distribution`, *pyro.distributions.torch_distribution.TorchDistributionMixin*

Base class for PyTorch-compatible distributions with Pyro support.

This should be the base class for almost all new Pyro distributions.

Note: Parameters and data should be of type `Tensor` and all methods return type `Tensor` unless otherwise noted.

Tensor Shapes:

TorchDistributions provide a method `.shape()` for the tensor shape of samples:

```
x = d.sample(sample_shape)
assert x.shape == d.shape(sample_shape)
```

Pyro follows the same distribution shape semantics as PyTorch. It distinguishes between three different roles for tensor shapes of samples:

- *sample shape* corresponds to the shape of the iid samples drawn from the distribution. This is taken as an argument by the distribution's *sample* method.
- *batch shape* corresponds to non-identical (independent) parameterizations of the distribution, inferred from the distribution's parameter shapes. This is fixed for a distribution instance.
- *event shape* corresponds to the event dimensions of the distribution, which is fixed for a distribution class. These are collapsed when we try to score a sample from the distribution via *d.log_prob(x)*.

These shapes are related by the equation:

```
assert d.shape(sample_shape) == sample_shape + d.batch_shape + d.event_shape
```

Distributions provide a vectorized `log_prob()` method that evaluates the log probability density of each event in a batch independently, returning a tensor of shape `sample_shape + d.batch_shape`:

```
x = d.sample(sample_shape)
assert x.shape == d.shape(sample_shape)
log_p = d.log_prob(x)
assert log_p.shape == sample_shape + d.batch_shape
```

Implementing New Distributions:

Derived classes must implement the methods `sample()` (or `rsample()` if `.has_rsample == True`) and `log_prob()`, and must implement the properties `batch_shape`, and `event_shape`. Discrete classes may also implement the `enumerate_support()` method to improve gradient estimates and set `.has_enumerate_support = True`.

expand(*batch_shape*, *_instance=None*)

Returns a new `ExpandedDistribution` instance with batch dimensions expanded to *batch_shape*.

Parameters

- **batch_shape** (*tuple*) – batch shape to expand to.

- **_instance** – unused argument for compatibility with `torch.distributions.Distribution.expand()`

Returns an instance of *ExpandedDistribution*.

Return type `ExpandedDistribution`

4.2.4 AVFMultivariateNormal

class AVFMultivariateNormal(*loc*, *scale_tril*, *control_var*)

Bases: `pyro.distributions.torch.MultivariateNormal`

Multivariate normal (Gaussian) distribution with transport equation inspired control variates (adaptive velocity fields).

A distribution over vectors in which all the elements have a joint Gaussian density.

Parameters

- **loc** (*torch.Tensor*) – D-dimensional mean vector.
- **scale_tril** (*torch.Tensor*) – Cholesky of Covariance matrix; D x D matrix.
- **control_var** (*torch.Tensor*) – 2 x L x D tensor that parameterizes the control variate; L is an arbitrary positive integer. This parameter needs to be learned (i.e. adapted) to achieve lower variance gradients. In a typical use case this parameter will be adapted concurrently with the *loc* and *scale_tril* that define the distribution.

Example usage:

```
control_var = torch.tensor(0.1 * torch.ones(2, 1, D), requires_grad=True)
opt_cv = torch.optim.Adam([control_var], lr=0.1, betas=(0.5, 0.999))

for _ in range(1000):
    d = AVFMultivariateNormal(loc, scale_tril, control_var)
    z = d.rsample()
    cost = torch.pow(z, 2.0).sum()
    cost.backward()
    opt_cv.step()
    opt_cv.zero_grad()
```

arg_constraints = {'control_var': Real(), 'loc': Real(), 'scale_tril': LowerTriangu

rsample(*sample_shape=torch.Size([])*)

4.2.5 BetaBinomial

class BetaBinomial(*concentration1*, *concentration0*, *total_count=1*, *validate_args=None*)

Bases: `pyro.distributions.torch_distribution.TorchDistribution`

Compound distribution comprising of a beta-binomial pair. The probability of success (`probs` for the *Binomial* distribution) is unknown and randomly drawn from a *Beta* distribution prior to a certain number of Bernoulli trials given by `total_count`.

Parameters

- **concentration1** (*float or torch.Tensor*) – 1st concentration parameter (alpha) for the Beta distribution.

- **concentration0** (*float or torch.Tensor*) – 2nd concentration parameter (beta) for the Beta distribution.
- **total_count** (*float or torch.Tensor*) – Number of Bernoulli trials.

approx_log_prob_tol = 0.0

arg_constraints = {'concentration0': GreaterThan(lower_bound=0.0), 'concentration1':

concentration0

concentration1

enumerate_support(*expand=True*)

expand(*batch_shape*, *_instance=None*)

has_enumerate_support = True

log_prob(*value*)

mean

sample(*sample_shape=()*)

support

variance

4.2.6 CoalescentTimes

class CoalescentTimes(*leaf_times*, *, *validate_args=None*)

Bases: pyro.distributions.torch_distribution.TorchDistribution

Distribution over coalescent times given irregular sampled `leaf_times`.

Sample values will be sorted sets of binary coalescent times. Each sample `value` will have cardinality `value.size(-1) = leaf_times.size(-1) - 1`, so that phylogenies are complete binary trees. This distribution can thus be batched over multiple samples of phylogenies given fixed (number of) leaf times, e.g. over phylogeny samples from BEAST or MrBayes.

References

[1] J.F.C. Kingman (1982) "On the Genealogy of Large Populations" Journal of Applied Probability

[2] J.F.C. Kingman (1982) "The Coalescent" Stochastic Processes and their Applications

Parameters **leaf_times** (*torch.Tensor*) – Vector of times of sampling events, i.e. leaf nodes in the phylogeny. These can be arbitrary real numbers with arbitrary order and duplicates.

arg_constraints = {'leaf_times': Real()}

log_prob(*value*)

sample(*sample_shape=torch.Size([])*)

support

4.2.7 CoalescentTimesWithRate

class CoalescentTimesWithRate(*leaf_times*, *rate_grid*, ***, *validate_args=None*)
Bases: pyro.distributions.torch_distribution.TorchDistribution

Distribution over coalescent times given irregular sampled `leaf_times` and piecewise constant coalescent rates defined on a regular time grid.

This assumes a piecewise constant base coalescent rate specified on time intervals `(-inf,1]`, `[1,2]`, ..., `[T-1,inf)`, where `T = rate_grid.size(-1)`. Leaves may be sampled at arbitrary real times, but are commonly sampled in the interval `[0, T]`.

Sample values will be sorted sets of binary coalescent times. Each sample `value` will have cardinality `value.size(-1) = leaf_times.size(-1) - 1`, so that phylogenies are complete binary trees. This distribution can thus be batched over multiple samples of phylogenies given fixed (number of) leaf times, e.g. over phylogeny samples from BEAST or MrBayes.

This distribution implements *log_prob()* but not `.sample()`.

See also *CoalescentRateLikelihood*.

References

[1] J.F.C. Kingman (1982) "On the Genealogy of Large Populations" Journal of Applied Probability

[2] J.F.C. Kingman (1982) "The Coalescent" Stochastic Processes and their Applications

[3] A. Popinga, T. Vaughan, T. Statler, A.J. Drummond (2014) "Inferring epidemiological dynamics with Bayesian coalescent inference: The merits of deterministic and stochastic models" https://arxiv.org/pdf/1407.1792.pdf

Parameters

- **leaf_times** (*torch.Tensor*) – Tensor of times of sampling events, i.e. leaf nodes in the phylogeny. These can be arbitrary real numbers with arbitrary order and duplicates.
- **rate_grid** (*torch.Tensor*) – Tensor of base coalescent rates (pairwise rate of coalescence). For example in a simple SIR model this might be `beta S / I`. The rightmost dimension is time, and this tensor represents a (batch of) rates that are piecwise constant in time.

arg_constraints = {'leaf_times': Real(), 'rate_grid': GreaterThan(lower_bound=0.0)}

duration

expand(*batch_shape*, *_instance=None*)

log_prob(*value*)
Computes likelihood as in equations 7-8 of [3].

This has time complexity `O(T + S N log(N))` where `T` is the number of time steps, `N` is the number of leaves, and `S = sample_shape.numel()` is the number of samples of `value`.

This is differentiable wrt `rate_grid` but neither `leaf_times` nor `value = coal_times`.

Parameters **value** (*torch.Tensor*) – A tensor of coalescent times. These denote sets of size `leaf_times.size(-1) - 1` along the trailing dimension and should be sorted along that dimension.

Returns Likelihood `p(coal_times | leaf_times, rate_grid)`

Return type torch.Tensor

support

4.2.8 ConditionalDistribution

class ConditionalDistribution
Bases: abc.ABC

condition(*context*)

Return type torch.distributions.Distribution

4.2.9 ConditionalTransformedDistribution

class ConditionalTransformedDistribution(*base_dist*, *transforms*)
Bases: pyro.distributions.conditional.ConditionalDistribution

clear_cache()

condition(*context*)

4.2.10 Delta

class Delta(*v*, *log_density=0.0*, *event_dim=0*, *validate_args=None*)
Bases: pyro.distributions.torch_distribution.TorchDistribution

Degenerate discrete distribution (a single point).

Discrete distribution that assigns probability one to the single element in its support. Delta distribution parameterized by a random choice should not be used with MCMC based inference, as doing so produces incorrect results.

Parameters

- **v** (*torch.Tensor*) – The single support element.
- **log_density** (*torch.Tensor*) – An optional density for this Delta. This is useful to keep the class of *Delta* distributions closed under differentiable transformation.
- **event_dim** (*int*) – Optional event dimension, defaults to zero.

arg_constraints = {'log_density': Real(), 'v': Real()}

expand(*batch_shape*, *_instance=None*)

has_rsample = True

log_prob(*x*)

mean

rsample(*sample_shape=torch.Size([])*)

support = Real()

variance

4.2.11 DirichletMultinomial

class DirichletMultinomial(*concentration*, *total_count=1*, *is_sparse=False*, *validate_args=None*)
Bases: pyro.distributions.torch_distribution.TorchDistribution

Compound distribution comprising of a dirichlet-multinomial pair. The probability of classes (`probs` for the *Multinomial* distribution) is unknown and randomly drawn from a *Dirichlet* distribution prior to a certain number of Categorical trials given by `total_count`.

Parameters

- **or torch.Tensor concentration** (*float*) – concentration parameter (alpha) for the Dirichlet distribution.
- **or torch.Tensor total_count** (*int*) – number of Categorical trials.
- **is_sparse** (*bool*) – Whether to assume value is mostly zero when computing *log_prob()*, which can speed up computation when data is sparse.

arg_constraints = {'concentration': GreaterThan(lower_bound=0.0), 'total_count': Int

concentration

expand(*batch_shape*, *_instance=None*)

log_prob(*value*)

mean

sample(*sample_shape=()*)

support

variance

4.2.12 DiscreteHMM

class DiscreteHMM(*initial_logits*, *transition_logits*, *observation_dist*, *validate_args=None*, *duration=None*)

Bases: `pyro.distributions.hmm.HiddenMarkovModel`

Hidden Markov Model with discrete latent state and arbitrary observation distribution. This uses [1] to parallelize over time, achieving O(log(time)) parallel complexity.

The event_shape of this distribution includes time on the left:

```
event_shape = (num_steps,) + observation_dist.event_shape
```

This distribution supports any combination of homogeneous/heterogeneous time dependency of `transition_logits` and `observation_dist`. However, because time is included in this distribution's event_shape, the homogeneous+homogeneous case will have a broadcastable event_shape with `num_steps = 1`, allowing *log_prob()* to work with arbitrary length data:

```
# homogeneous + homogeneous case:
event_shape = (1,) + observation_dist.event_shape
```

References:

[1] Simo Sarkka, Angel F. Garcia-Fernandez (2019) "Temporal Parallelization of Bayesian Filters and Smoothers" https://arxiv.org/pdf/1905.13002.pdf

Parameters

- **initial_logits** (*Tensor*) – A logits tensor for an initial categorical distribution over latent states. Should have rightmost size `state_dim` and be broadcastable to `batch_shape + (state_dim,)`.

- **transition_logits** (*Tensor*) – A logits tensor for transition conditional distributions between latent states. Should have rightmost shape `(state_dim, state_dim)` (old, new), and be broadcastable to `batch_shape + (num_steps, state_dim, state_dim)`.
- **observation_dist** (*Distribution*) – A conditional distribution of observed data conditioned on latent state. The `.batch_shape` should have rightmost size `state_dim` and be broadcastable to `batch_shape + (num_steps, state_dim)`. The `.event_shape` may be arbitrary.
- **duration** (*int*) – Optional size of the time axis `event_shape[0]`. This is required when sampling from homogeneous HMMs whose parameters are not expanded along the time axis.

arg_constraints = {'initial_logits': Real(), 'transition_logits': Real()}

expand(*batch_shape*, *_instance=None*)

filter(*value*)

Compute posterior over final state given a sequence of observations.

Parameters **value** (*Tensor*) – A sequence of observations.

Returns A posterior distribution over latent states at the final time step. `result.logits` can then be used as `initial_logits` in a sequential Pyro model for prediction.

Return type *Categorical*

log_prob(*value*)

support

4.2.13 EmpiricalDistribution

class Empirical(*samples*, *log_weights*, *validate_args=None*)

Bases: `pyro.distributions.torch_distribution.TorchDistribution`

Empirical distribution associated with the sampled data. Note that the shape requirement for *log_weights* is that its shape must match the leftmost shape of *samples*. Samples are aggregated along the `aggregation_dim`, which is the rightmost dim of *log_weights*.

Example:

```
>>> emp_dist = Empirical(torch.randn(2, 3, 10), torch.ones(2, 3))
>>> emp_dist.batch_shape
torch.Size([2])
>>> emp_dist.event_shape
torch.Size([10])
```

```
>>> single_sample = emp_dist.sample()
>>> single_sample.shape
torch.Size([2, 10])
>>> batch_sample = emp_dist.sample((100,))
>>> batch_sample.shape
torch.Size([100, 2, 10])
```

```
>>> emp_dist.log_prob(single_sample).shape
torch.Size([2])
```

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```
>>> # Vectorized samples cannot be scored by log_prob.
>>> with pyro.validation_enabled():
...     emp_dist.log_prob(batch_sample).shape
Traceback (most recent call last):
...
ValueError: ``value.shape`` must be torch.Size([2, 10])
```

Parameters

- **samples** (*torch.Tensor*) – samples from the empirical distribution.
- **log_weights** (*torch.Tensor*) – log weights (optional) corresponding to the samples.

arg_constraints = {}

enumerate_support(*expand=True*)
See pyro.distributions.torch_distribution.TorchDistribution.enumerate_support()

event_shape
See pyro.distributions.torch_distribution.TorchDistribution.event_shape()

has_enumerate_support = True

log_prob(*value*)
Returns the log of the probability mass function evaluated at value. Note that this currently only supports scoring values with empty sample_shape.

Parameters **value** (*torch.Tensor*) – scalar or tensor value to be scored.

log_weights

mean
See pyro.distributions.torch_distribution.TorchDistribution.mean()

sample(*sample_shape=torch.Size([])*)
See pyro.distributions.torch_distribution.TorchDistribution.sample()

sample_size
Number of samples that constitute the empirical distribution.

Return int number of samples collected.

support = Real()

variance
See pyro.distributions.torch_distribution.TorchDistribution.variance()

4.2.14 ExtendedBetaBinomial

class ExtendedBetaBinomial(*concentration1*, *concentration0*, *total_count=1*, *validate_args=None*)
Bases: pyro.distributions.conjugate.BetaBinomial

EXPERIMENTAL *BetaBinomial* distribution extended to have logical support the entire integers and to allow arbitrary integer total_count. Numerical support is still the integer interval [0, total_count].

arg_constraints = {'concentration0': GreaterThan(lower_bound=0.0), 'concentration1':

log_prob(*value*)

support = Integer

4.2.15 ExtendedBinomial

class ExtendedBinomial(*total_count=1*, *probs=None*, *logits=None*, *validate_args=None*)
Bases: pyro.distributions.torch.Binomial

EXPERIMENTAL *Binomial* distribution extended to have logical support the entire integers and to allow arbitrary integer total_count. Numerical support is still the integer interval [0, total_count].

arg_constraints = {'logits': Real(), 'probs': Interval(lower_bound=0.0, upper_bound=

log_prob(*value*)

support = Integer

4.2.16 FoldedDistribution

class FoldedDistribution(*base_dist*, *validate_args=None*)
Bases: pyro.distributions.torch.TransformedDistribution

Equivalent to TransformedDistribution(base_dist, AbsTransform()), but additionally supports *log_prob()* .

Parameters **base_dist** (*Distribution*) – The distribution to reflect.

expand(*batch_shape*, *_instance=None*)

log_prob(*value*)

support = GreaterThan(lower_bound=0.0)

4.2.17 GammaGaussianHMM

class GammaGaussianHMM(*scale_dist*, *initial_dist*, *transition_matrix*, *transition_dist*, *observation_matrix*, *observation_dist*, *validate_args=None*, *duration=None*)
Bases: pyro.distributions.hmm.HiddenMarkovModel

Hidden Markov Model with the joint distribution of initial state, hidden state, and observed state is a *MultivariateStudentT* distribution along the line of references [2] and [3]. This adapts [1] to parallelize over time to achieve O(log(time)) parallel complexity.

This GammaGaussianHMM class corresponds to the generative model:

```
s = Gamma(df/2, df/2).sample()
z = scale(initial_dist, s).sample()
x = []
for t in range(num_events):
    z = z @ transition_matrix + scale(transition_dist, s).sample()
    x.append(z @ observation_matrix + scale(observation_dist, s).sample())
```

where *scale(mvn(loc, precision), s) := mvn(loc, s * precision)*.

The event_shape of this distribution includes time on the left:

```
event_shape = (num_steps,) + observation_dist.event_shape
```

This distribution supports any combination of homogeneous/heterogeneous time dependency of `transition_dist` and `observation_dist`. However, because time is included in this distribution's event_shape, the homogeneous+homogeneous case will have a broadcastable event_shape with `num_steps = 1`, allowing *log_prob()* to work with arbitrary length data:

```
event_shape = (1, obs_dim)  # homogeneous + homogeneous case
```

References:

[1] Simo Sarkka, Angel F. Garcia-Fernandez (2019) "Temporal Parallelization of Bayesian Filters and Smoothers" https://arxiv.org/pdf/1905.13002.pdf

[2] F. J. Giron and J. C. Rojano (1994) "Bayesian Kalman filtering with elliptically contoured errors"

[3] Filip Tronarp, Toni Karvonen, and Simo Sarkka (2019) "Student's t-filters for noise scale estimation" https://users.aalto.fi/~ssarkka/pub/SPL2019.pdf

Variables

- **hidden_dim** (*int*) – The dimension of the hidden state.
- **obs_dim** (*int*) – The dimension of the observed state.

Parameters

- **scale_dist** (Gamma) – Prior of the mixing distribution.
- **initial_dist** (MultivariateNormal) – A distribution with unit scale mixing over initial states. This should have batch_shape broadcastable to `self.batch_shape`. This should have event_shape `(hidden_dim,)`.
- **transition_matrix** (*Tensor*) – A linear transformation of hidden state. This should have shape broadcastable to `self.batch_shape + (num_steps, hidden_dim, hidden_dim)` where the rightmost dims are ordered `(old, new)`.
- **transition_dist** (MultivariateNormal) – A process noise distribution with unit scale mixing. This should have batch_shape broadcastable to `self.batch_shape + (num_steps,)`. This should have event_shape `(hidden_dim,)`.
- **observation_matrix** (*Tensor*) – A linear transformation from hidden to observed state. This should have shape broadcastable to `self.batch_shape + (num_steps, hidden_dim, obs_dim)`.
- **observation_dist** (MultivariateNormal) – An observation noise distribution with unit scale mixing. This should have batch_shape broadcastable to `self.batch_shape + (num_steps,)`. This should have event_shape `(obs_dim,)`.
- **duration** (*int*) – Optional size of the time axis `event_shape[0]`. This is required when sampling from homogeneous HMMs whose parameters are not expanded along the time axis.

arg_constraints = {}

expand(*batch_shape*, *_instance=None*)

filter(*value*)

Compute posteriors over the multiplier and the final state given a sequence of observations. The posterior is a pair of Gamma and MultivariateNormal distributions (i.e. a GammaGaussian instance).

Parameters **value** (*Tensor*) – A sequence of observations.

Returns A pair of posterior distributions over the mixing and the latent state at the final time step.

Return type a tuple of ~pyro.distributions.Gamma and ~pyro.distributions.MultivariateNormal

log_prob(*value*)

support = Real()

4.2.18 GammaPoisson

class GammaPoisson(*concentration*, *rate*, *validate_args=None*)

Bases: pyro.distributions.torch_distribution.TorchDistribution

Compound distribution comprising of a gamma-poisson pair, also referred to as a gamma-poisson mixture. The rate parameter for the *Poisson* distribution is unknown and randomly drawn from a *Gamma* distribution.

Note: This can be treated as an alternate parametrization of the *NegativeBinomial* (total_count, probs) distribution, with *concentration* = *total_count* and *rate* = *(1 - probs) / probs*.

Parameters

- **or torch.Tensor concentration** (*float*) – shape parameter (alpha) of the Gamma distribution.
- **or torch.Tensor rate** (*float*) – rate parameter (beta) for the Gamma distribution.

arg_constraints = {'concentration': GreaterThan(lower_bound=0.0), 'rate': GreaterThan

concentration

expand(*batch_shape*, *_instance=None*)

log_prob(*value*)

mean

rate

sample(*sample_shape=()*)

support = IntegerGreaterThan(lower_bound=0)

variance

4.2.19 GaussianHMM

class GaussianHMM(*initial_dist*, *transition_matrix*, *transition_dist*, *observation_matrix*, *observation_dist*, *validate_args=None*, *duration=None*)

Bases: pyro.distributions.hmm.HiddenMarkovModel

Hidden Markov Model with Gaussians for initial, transition, and observation distributions. This adapts [1] to parallelize over time to achieve O(log(time)) parallel complexity, however it differs in that it tracks the log normalizer to ensure *log_prob()* is differentiable.

This corresponds to the generative model:

```
z = initial_distribution.sample()
x = []
for t in range(num_events):
    z = z @ transition_matrix + transition_dist.sample()
    x.append(z @ observation_matrix + observation_dist.sample())
```

The event_shape of this distribution includes time on the left:

```
event_shape = (num_steps,) + observation_dist.event_shape
```

This distribution supports any combination of homogeneous/heterogeneous time dependency of `transition_dist` and `observation_dist`. However, because time is included in this distribution's event_shape, the homogeneous+homogeneous case will have a broadcastable event_shape with `num_steps = 1`, allowing *log_prob()* to work with arbitrary length data:

```
event_shape = (1, obs_dim)  # homogeneous + homogeneous case
```

References:

[1] Simo Sarkka, Angel F. Garcia-Fernandez (2019) "Temporal Parallelization of Bayesian Filters and Smoothers" https://arxiv.org/pdf/1905.13002.pdf

Variables

- **hidden_dim** (*int*) – The dimension of the hidden state.
- **obs_dim** (*int*) – The dimension of the observed state.

Parameters

- **initial_dist** (*MultivariateNormal*) – A distribution over initial states. This should have batch_shape broadcastable to `self.batch_shape`. This should have event_shape `(hidden_dim,)`.
- **transition_matrix** (*Tensor*) – A linear transformation of hidden state. This should have shape broadcastable to `self.batch_shape + (num_steps, hidden_dim, hidden_dim)` where the rightmost dims are ordered `(old, new)`.
- **transition_dist** (*MultivariateNormal*) – A process noise distribution. This should have batch_shape broadcastable to `self.batch_shape + (num_steps,)`. This should have event_shape `(hidden_dim,)`.
- **observation_matrix** (*Tensor*) – A linear transformation from hidden to observed state. This should have shape broadcastable to `self.batch_shape + (num_steps, hidden_dim, obs_dim)`.
- **observation_dist** (*MultivariateNormal or Normal*) – An observation noise distribution. This should have batch_shape broadcastable to `self.batch_shape + (num_steps,)`. This should have event_shape `(obs_dim,)`.
- **duration** (*int*) – Optional size of the time axis `event_shape[0]`. This is required when sampling from homogeneous HMMs whose parameters are not expanded along the time axis.

arg_constraints = {}

conjugate_update(*other*)

EXPERIMENTAL Creates an updated *GaussianHMM* fusing information from another compatible distribution.

This should satisfy:

```
fg, log_normalizer = f.conjugate_update(g)
assert f.log_prob(x) + g.log_prob(x) == fg.log_prob(x) + log_normalizer
```

Parameters **other** (*MultivariateNormal or Normal*) – A distribution representing `p(data|self.probs)` but normalized over `self.probs` rather than `data`.

Returns a pair `(updated,log_normalizer)` where `updated` is an updated *GaussianHMM* , and `log_normalizer` is a `Tensor` representing the normalization factor.

expand(*batch_shape*, *_instance=None*)

filter(*value*)

Compute posterior over final state given a sequence of observations.

Parameters **value** (*Tensor*) – A sequence of observations.

Returns A posterior distribution over latent states at the final time step. `result` can then be used as `initial_dist` in a sequential Pyro model for prediction.

Return type *MultivariateNormal*

has_rsample = True

log_prob(*value*)

prefix_condition(*data*)

EXPERIMENTAL Given self has `event_shape == (t+f, d)` and data `x` of shape `batch_shape + (t, d)`, compute a conditional distribution of event_shape `(f, d)`. Typically `t` is the number of training time steps, `f` is the number of forecast time steps, and `d` is the data dimension.

Parameters **data** (*Tensor*) – data of dimension at least 2.

rsample(*sample_shape=torch.Size([])*)

rsample_posterior(*value*, *sample_shape=torch.Size([])*)

EXPERIMENTAL Sample from the latent state conditioned on observation.

support = Real()

4.2.20 GaussianMRF

class GaussianMRF(*initial_dist*, *transition_dist*, *observation_dist*, *validate_args=None*)

Bases: `pyro.distributions.torch_distribution.TorchDistribution`

Temporal Markov Random Field with Gaussian factors for initial, transition, and observation distributions. This adapts [1] to parallelize over time to achieve O(log(time)) parallel complexity, however it differs in that it tracks the log normalizer to ensure *log_prob()* is differentiable.

The event_shape of this distribution includes time on the left:

```
event_shape = (num_steps,) + observation_dist.event_shape
```

This distribution supports any combination of homogeneous/heterogeneous time dependency of `transition_dist` and `observation_dist`. However, because time is included in this distribution's event_shape, the homogeneous+homogeneous case will have a broadcastable event_shape with `num_steps = 1`, allowing *log_prob()* to work with arbitrary length data:

```
event_shape = (1, obs_dim)  # homogeneous + homogeneous case
```

References:

[1] Simo Sarkka, Angel F. Garcia-Fernandez (2019) "Temporal Parallelization of Bayesian Filters and Smoothers" https://arxiv.org/pdf/1905.13002.pdf

Variables

- **hidden_dim** (*int*) – The dimension of the hidden state.
- **obs_dim** (*int*) – The dimension of the observed state.

Parameters

- **initial_dist** (*MultivariateNormal*) – A distribution over initial states. This should have batch_shape broadcastable to `self.batch_shape`. This should have event_shape `(hidden_dim,)`.
- **transition_dist** (*MultivariateNormal*) – A joint distribution factor over a pair of successive time steps. This should have batch_shape broadcastable to `self.batch_shape + (num_steps,)`. This should have event_shape `(hidden_dim + hidden_dim,)` (old+new).
- **observation_dist** (*MultivariateNormal*) – A joint distribution factor over a hidden and an observed state. This should have batch_shape broadcastable to `self.batch_shape + (num_steps,)`. This should have event_shape `(hidden_dim + obs_dim,)`.

arg_constraints = {}

expand(*batch_shape*, *_instance=None*)

log_prob(*value*)

4.2.21 GaussianScaleMixture

class GaussianScaleMixture(*coord_scale*, *component_logits*, *component_scale*)

Bases: `pyro.distributions.torch_distribution.TorchDistribution`

Mixture of Normal distributions with zero mean and diagonal covariance matrices.

That is, this distribution is a mixture with K components, where each component distribution is a D-dimensional Normal distribution with zero mean and a D-dimensional diagonal covariance matrix. The K different covariance matrices are controlled by the parameters *coord_scale* and *component_scale*. That is, the covariance matrix of the k'th component is given by

Sigma_ii = (component_scale_k * coord_scale_i) ** 2 (i = 1, . . . , D)

where *component_scale_k* is a positive scale factor and *coord_scale_i* are positive scale parameters shared between all K components. The mixture weights are controlled by a K-dimensional vector of softmax logits, *component_logits*. This distribution implements pathwise derivatives for samples from the distribution. This distribution does not currently support batched parameters.

See reference [1] for details on the implementations of the pathwise derivative. Please consider citing this reference if you use the pathwise derivative in your research.

[1] Pathwise Derivatives for Multivariate Distributions, Martin Jankowiak & Theofanis Karaletsos. arXiv:1806.01856

Note that this distribution supports both even and odd dimensions, but the former should be more a bit higher precision, since it doesn't use any erfs in the backward call. Also note that this distribution does not support D = 1.

Parameters

- **coord_scale** (*torch.tensor*) – D-dimensional vector of scales
- **component_logits** (*torch.tensor*) – K-dimensional vector of logits

- **component_scale** (*torch.tensor*) – K-dimensional vector of scale multipliers

arg_constraints = {'component_logits': Real(), 'component_scale': GreaterThan(lower_

has_rsample = True

log_prob(*value*)

rsample(*sample_shape=torch.Size([])*)

4.2.22 ImproperUniform

class ImproperUniform(*support*, *batch_shape*, *event_shape*)

Bases: pyro.distributions.torch_distribution.TorchDistribution

Improper distribution with zero *log_prob()* and undefined *sample()*.

This is useful for transforming a model from generative dag form to factor graph form for use in HMC. For example the following are equal in distribution:

```
# Version 1. a generative dag
x = pyro.sample("x", Normal(0, 1))
y = pyro.sample("y", Normal(x, 1))
z = pyro.sample("z", Normal(y, 1))

# Version 2. a factor graph
xyz = pyro.sample("xyz", ImproperUniform(constraints.real, (), (3,)))
x, y, z = xyz.unbind(-1)
pyro.sample("x", Normal(0, 1), obs=x)
pyro.sample("y", Normal(x, 1), obs=y)
pyro.sample("z", Normal(y, 1), obs=z)
```

Note this distribution errors when *sample()* is called. To create a similar distribution that instead samples from a specified distribution consider using `.mask(False)` as in:

```
xyz = dist.Normal(0, 1).expand([3]).to_event(1).mask(False)
```

Parameters

- **support** (*Constraint*) – The support of the distribution.
- **batch_shape** (*torch.Size*) – The batch shape.
- **event_shape** (*torch.Size*) – The event shape.

arg_constraints = {}

expand(*batch_shape*, *_instance=None*)

log_prob(*value*)

sample(*sample_shape=torch.Size([])*)

support

4.2.23 IndependentHMM

class IndependentHMM(*base_dist*)

Bases: pyro.distributions.torch_distribution.TorchDistribution

Wrapper class to treat a batch of independent univariate HMMs as a single multivariate distribution. This converts distribution shapes as follows:

	.batch_shape	.event_shape
base_dist	shape + (obs_dim,)	(duration, 1)
result	shape	(duration, obs_dim)

Parameters **base_dist** (*HiddenMarkovModel*) – A base hidden Markov model instance.

arg_constraints = {}

duration

expand(*batch_shape*, *_instance=None*)

has_rsample

log_prob(*value*)

rsample(*sample_shape=torch.Size([])*)

support

4.2.24 InverseGamma

class InverseGamma(*concentration*, *rate*, *validate_args=None*)
Bases: pyro.distributions.torch.TransformedDistribution

Creates an inverse-gamma distribution parameterized by *concentration* and *rate*.

X ~ Gamma(concentration, rate) Y = 1/X ~ InverseGamma(concentration, rate)

Parameters

- **concentration** (*torch.Tensor*) – the concentration parameter (i.e. alpha).
- **rate** (*torch.Tensor*) – the rate parameter (i.e. beta).

arg_constraints = {'concentration': GreaterThan(lower_bound=0.0), 'rate': GreaterTha

concentration

expand(*batch_shape*, *_instance=None*)

has_rsample = True

rate

support = GreaterThan(lower_bound=0.0)

4.2.25 LinearHMM

class LinearHMM(*initial_dist*, *transition_matrix*, *transition_dist*, *observation_matrix*, *observation_dist*, *validate_args=None*, *duration=None*)
Bases: pyro.distributions.hmm.HiddenMarkovModel

Hidden Markov Model with linear dynamics and observations and arbitrary noise for initial, transition, and observation distributions. Each of those distributions can be e.g. *MultivariateNormal* or *Independent* of *Normal*, *StudentT*, or *Stable* . Additionally the observation distribution may be constrained, e.g. *LogNormal*

This corresponds to the generative model:

```
z = initial_distribution.sample()
x = []
for t in range(num_events):
    z = z @ transition_matrix + transition_dist.sample()
    y = z @ observation_matrix + obs_base_dist.sample()
    x.append(obs_transform(y))
```

where `observation_dist` is split into `obs_base_dist` and an optional `obs_transform` (defaulting to the identity).

This implements a reparameterized *`rsample()`* method but does not implement a *`log_prob()`* method. Derived classes may implement *`log_prob()`* .

Inference without *`log_prob()`* can be performed using either reparameterization with *`LinearHMMReparam`* or likelihood-free algorithms such as *`EnergyDistance`* . Note that while stable processes generally require a common shared stability parameter α , this distribution and the above inference algorithms allow heterogeneous stability parameters.

The event_shape of this distribution includes time on the left:

```
event_shape = (num_steps,) + observation_dist.event_shape
```

This distribution supports any combination of homogeneous/heterogeneous time dependency of `transition_dist` and `observation_dist`. However at least one of the distributions or matrices must be expanded to contain the time dimension.

Variables

- **`hidden_dim`** (*`int`*) – The dimension of the hidden state.
- **`obs_dim`** (*`int`*) – The dimension of the observed state.

Parameters

- **`initial_dist`** – A distribution over initial states. This should have batch_shape broadcastable to `self.batch_shape`. This should have event_shape `(hidden_dim,)`.
- **`transition_matrix`** (*`Tensor`*) – A linear transformation of hidden state. This should have shape broadcastable to `self.batch_shape + (num_steps, hidden_dim, hidden_dim)` where the rightmost dims are ordered `(old, new)`.
- **`transition_dist`** – A distribution over process noise. This should have batch_shape broadcastable to `self.batch_shape + (num_steps,)`. This should have event_shape `(hidden_dim,)`.
- **`observation_matrix`** (*`Tensor`*) – A linear transformation from hidden to observed state. This should have shape broadcastable to `self.batch_shape + (num_steps, hidden_dim, obs_dim)`.
- **`observation_dist`** – A observation noise distribution. This should have batch_shape broadcastable to `self.batch_shape + (num_steps,)`. This should have event_shape `(obs_dim,)`.
- **`duration`** (*`int`*) – Optional size of the time axis `event_shape[0]`. This is required when sampling from homogeneous HMMs whose parameters are not expanded along the time axis.

`arg_constraints = {}`

`expand`(*batch_shape*, *_instance=None*)

has_rsample = True

log_prob(*value*)

rsample(*sample_shape=torch.Size([])*)

support

4.2.26 LKJCorrCholesky

class LKJCorrCholesky(*d*, *eta*, *validate_args=None*)
Bases: pyro.distributions.torch_distribution.TorchDistribution

Generates cholesky factors of correlation matrices using an LKJ prior.

The expected use is to combine it with a vector of variances and pass it to the scale_tril parameter of a multivariate distribution such as MultivariateNormal.

E.g., if theta is a (positive) vector of covariances with the same dimensionality as this distribution, and Omega is sampled from this distribution, scale_tril=torch.mm(torch.diag(sqrt(theta)), Omega)

Note that the *event_shape* of this distribution is *[d, d]*

Note: When using this distribution with HMC/NUTS, it is important to use a *step_size* such as 1e-4. If not, you are likely to experience LAPACK errors regarding positive-definiteness.

For example usage, refer to pyro/examples/lkj.py.

Parameters

- **d** (*int*) – Dimensionality of the matrix
- **eta** (*torch.Tensor*) – A single positive number parameterizing the distribution.

arg_constraints = {'eta': GreaterThan(lower_bound=0.0)}

expand(*batch_shape*, *_instance=None*)

has_rsample = False

lkj_constant(*eta*, *K*)

log_prob(*x*)

sample(*sample_shape=torch.Size([])*)

support = CorrCholesky()

4.2.27 MaskedDistribution

class MaskedDistribution(*base_dist*, *mask*)
Bases: pyro.distributions.torch_distribution.TorchDistribution

Masks a distribution by a boolean tensor that is broadcastable to the distribution's `batch_shape`.

In the special case `mask is False`, computation of *log_prob()* , *score_parts()* , and `kl_divergence()` is skipped, and constant zero values are returned instead.

Parameters **mask** (*torch.Tensor or bool*) – A boolean or boolean-valued tensor.

arg_constraints = {}

conjugate_update(*other*)
EXPERIMENTAL.

enumerate_support(*expand=True*)

expand(*batch_shape*, *_instance=None*)

has_enumerate_support

has_rsample

log_prob(*value*)

mean

rsample(*sample_shape=torch.Size([])*)

sample(*sample_shape=torch.Size([])*)

score_parts(*value*)

support

variance

4.2.28 MaskedMixture

class MaskedMixture(*mask*, *component0*, *component1*, *validate_args=None*)
Bases: `pyro.distributions.torch_distribution.TorchDistribution`

A masked deterministic mixture of two distributions.

This is useful when the mask is sampled from another distribution, possibly correlated across the batch. Often the mask can be marginalized out via enumeration.

Example:

```
change_point = pyro.sample("change_point",
                           dist.Categorical(torch.ones(len(data) + 1)),
                           infer={'enumerate': 'parallel'})
mask = torch.arange(len(data), dtype=torch.long) >= changepoint
with pyro.plate("data", len(data)):
    pyro.sample("obs", MaskedMixture(mask, dist1, dist2), obs=data)
```

Parameters

- **mask** (*torch.Tensor*) – A boolean tensor toggling between `component0` and `component1`.
- **component0** (`pyro.distributions.TorchDistribution`) – a distribution for batch elements `mask == False`.
- **component1** (`pyro.distributions.TorchDistribution`) – a distribution for batch elements `mask == True`.

arg_constraints = {}

expand(*batch_shape*)

has_rsample

log_prob(*value*)

mean

rsample(*sample_shape=torch.Size([])*)

sample(*sample_shape=torch.Size([])*)

support

variance

4.2.29 MixtureOfDiagNormals

class MixtureOfDiagNormals(*locs*, *coord_scale*, *component_logits*)
Bases: pyro.distributions.torch_distribution.TorchDistribution

Mixture of Normal distributions with arbitrary means and arbitrary diagonal covariance matrices.

That is, this distribution is a mixture with K components, where each component distribution is a D-dimensional Normal distribution with a D-dimensional mean parameter and a D-dimensional diagonal covariance matrix. The K different component means are gathered into the K x D dimensional parameter *locs* and the K different scale parameters are gathered into the K x D dimensional parameter *coord_scale*. The mixture weights are controlled by a K-dimensional vector of softmax logits, *component_logits*. This distribution implements pathwise derivatives for samples from the distribution.

See reference [1] for details on the implementations of the pathwise derivative. Please consider citing this reference if you use the pathwise derivative in your research. Note that this distribution does not support dimension D = 1.

[1] Pathwise Derivatives for Multivariate Distributions, Martin Jankowiak & Theofanis Karaletsos. arXiv:1806.01856

Parameters

- **locs** (*torch.Tensor*) – K x D mean matrix
- **coord_scale** (*torch.Tensor*) – K x D scale matrix
- **component_logits** (*torch.Tensor*) – K-dimensional vector of softmax logits

arg_constraints = {'component_logits': Real(), 'coord_scale': GreaterThan(lower_boun

expand(*batch_shape*, *_instance=None*)

has_rsample = True

log_prob(*value*)

rsample(*sample_shape=torch.Size([])*)

4.2.30 MixtureOfDiagNormalsSharedCovariance

class MixtureOfDiagNormalsSharedCovariance(*locs*, *coord_scale*, *component_logits*)
Bases: pyro.distributions.torch_distribution.TorchDistribution

Mixture of Normal distributions with diagonal covariance matrices.

That is, this distribution is a mixture with K components, where each component distribution is a D-dimensional Normal distribution with a D-dimensional mean parameter loc and a D-dimensional diagonal covariance matrix specified by a scale parameter *coord_scale*. The K different component means are gathered into the parameter *locs* and the scale parameter is shared between all K components. The mixture weights are controlled by a K-dimensional vector of softmax logits, *component_logits*. This distribution implements pathwise derivatives for samples from the distribution.

See reference [1] for details on the implementations of the pathwise derivative. Please consider citing this reference if you use the pathwise derivative in your research. Note that this distribution does not support dimension D = 1.

[1] Pathwise Derivatives for Multivariate Distributions, Martin Jankowiak & Theofanis Karaletsos. arXiv:1806.01856

Parameters

- **locs** (*torch.Tensor*) – K x D mean matrix
- **coord_scale** (*torch.Tensor*) – shared D-dimensional scale vector
- **component_logits** (*torch.Tensor*) – K-dimensional vector of softmax logits

arg_constraints = {'component_logits': Real(), 'coord_scale': GreaterThan(lower_boun

expand(*batch_shape*, *_instance=None*)

has_rsample = True

log_prob(*value*)

rsample(*sample_shape=torch.Size([])*)

4.2.31 MultivariateStudentT

class MultivariateStudentT(*df*, *loc*, *scale_tril*, *validate_args=None*)

Bases: pyro.distributions.torch_distribution.TorchDistribution

Creates a multivariate Student's t-distribution parameterized by degree of freedom `df`, mean `loc` and scale *scale_tril*.

Parameters

- **df** (*Tensor*) – degrees of freedom
- **loc** (*Tensor*) – mean of the distribution
- **scale_tril** (*Tensor*) – scale of the distribution, which is a lower triangular matrix with positive diagonal entries

arg_constraints = {'df': GreaterThan(lower_bound=0.0), 'loc': RealVector(), 'scale_t

covariance_matrix

expand(*batch_shape*, *_instance=None*)

has_rsample = True

log_prob(*value*)

mean

precision_matrix

rsample(*sample_shape=torch.Size([])*)

scale_tril

support = RealVector()

variance

4.2.32 OMTMultivariateNormal

class OMTMultivariateNormal(*loc*, *scale_tril*)
Bases: pyro.distributions.torch.MultivariateNormal

Multivariate normal (Gaussian) distribution with OMT gradients w.r.t. both parameters. Note the gradient computation w.r.t. the Cholesky factor has cost O(D^3), although the resulting gradient variance is generally expected to be lower.

A distribution over vectors in which all the elements have a joint Gaussian density.

Parameters

- **loc** (*torch.Tensor*) – Mean.
- **scale_tril** (*torch.Tensor*) – Cholesky of Covariance matrix.

arg_constraints = {'loc': Real(), 'scale_tril': LowerTriangular()}

rsample(*sample_shape=torch.Size([])*)

4.2.33 OrderedLogistic

class OrderedLogistic(*predictor*, *cutpoints*, *validate_args=None*)
Bases: pyro.distributions.torch.Categorical

Alternative parametrization of the distribution over a categorical variable.

Instead of the typical parametrization of a categorical variable in terms of the probability mass of the individual categories `p`, this provides an alternative that is useful in specifying ordered categorical models. This accepts a vector of `cutpoints` which are an ordered vector of real numbers denoting baseline cumulative log-odds of the individual categories, and a model vector `predictor` which modifies the baselines for each sample individually.

These cumulative log-odds are then transformed into a discrete cumulative probability distribution, that is finally differenced to return the probability mass matrix `p` that specifies the categorical distribution.

Parameters

- **predictor** (*Tensor*) – A tensor of predictor variables of arbitrary shape. The output shape of non-batched samples from this distribution will be the same shape as `predictor`.
- **cutpoints** (*Tensor*) – A tensor of cutpoints that are used to determine the cumulative probability of each entry in `predictor` belonging to a given category. The first *cutpoints.ndim-1* dimensions must be broadcastable to `predictor`, and the -1 dimension is monotonically increasing.

arg_constraints = {'cutpoints': OrderedVector(), 'predictor': Real()}

expand(*batch_shape*, *_instance=None*)

4.2.34 RelaxedBernoulliStraightThrough

class RelaxedBernoulliStraightThrough(*temperature*, *probs=None*, *logits=None*, *validate_args=None*)
Bases: pyro.distributions.torch.RelaxedBernoulli

An implementation of `RelaxedBernoulli` with a straight-through gradient estimator.

This distribution has the following properties:

- The samples returned by the *rsample()* method are discrete/quantized.
- The *log_prob()* method returns the log probability of the relaxed/unquantized sample using the GumbelSoftmax distribution.
- In the backward pass the gradient of the sample with respect to the parameters of the distribution uses the relaxed/unquantized sample.

References:

[1] The Concrete Distribution: A Continuous Relaxation of Discrete Random Variables, Chris J. Maddison, Andriy Mnih, Yee Whye Teh

[2] Categorical Reparameterization with Gumbel-Softmax, Eric Jang, Shixiang Gu, Ben Poole

log_prob(*value*)
See pyro.distributions.torch.RelaxedBernoulli.log_prob()

rsample(*sample_shape=torch.Size([])*)
See pyro.distributions.torch.RelaxedBernoulli.rsample()

4.2.35 RelaxedOneHotCategoricalStraightThrough

class RelaxedOneHotCategoricalStraightThrough(*temperature*, *probs=None*, *logits=None*, *validate_args=None*)
Bases: pyro.distributions.torch.RelaxedOneHotCategorical

An implementation of RelaxedOneHotCategorical with a straight-through gradient estimator.

This distribution has the following properties:

- The samples returned by the *rsample()* method are discrete/quantized.
- The *log_prob()* method returns the log probability of the relaxed/unquantized sample using the GumbelSoftmax distribution.
- In the backward pass the gradient of the sample with respect to the parameters of the distribution uses the relaxed/unquantized sample.

References:

[1] The Concrete Distribution: A Continuous Relaxation of Discrete Random Variables, Chris J. Maddison, Andriy Mnih, Yee Whye Teh

[2] Categorical Reparameterization with Gumbel-Softmax, Eric Jang, Shixiang Gu, Ben Poole

log_prob(*value*)
See pyro.distributions.torch.RelaxedOneHotCategorical.log_prob()

rsample(*sample_shape=torch.Size([])*)
See pyro.distributions.torch.RelaxedOneHotCategorical.rsample()

4.2.36 Rejector

class Rejector(*propose*, *log_prob_accept*, *log_scale*, *, *batch_shape=None*, *event_shape=None*)
Bases: pyro.distributions.torch_distribution.TorchDistribution

Rejection sampled distribution given an acceptance rate function.

Parameters

- **propose** (Distribution) – A proposal distribution that samples batched proposals via `propose().rsample()` supports a `sample_shape` arg only if `propose()` supports a `sample_shape` arg.
- **log_prob_accept** (*callable*) – A callable that inputs a batch of proposals and returns a batch of log acceptance probabilities.
- **log_scale** – Total log probability of acceptance.

arg_constraints = {}

has_rsample = True

log_prob(*x*)

rsample(*sample_shape=torch.Size([])*)

score_parts(*x*)

4.2.37 SpanningTree

class SpanningTree(*edge_logits*, *sampler_options=None*, *validate_args=None*)

Bases: `pyro.distributions.torch_distribution.TorchDistribution`

Distribution over spanning trees on a fixed number `V` of vertices.

A tree is represented as `torch.LongTensor edges` of shape `(V-1,2)` satisfying the following properties:

1. The edges constitute a tree, i.e. are connected and cycle free.
2. Each edge `(v1,v2) = edges[e]` is sorted, i.e. `v1 < v2`.
3. The entire tensor is sorted in colexicographic order.

Use *validate_edges()* to verify *edges* are correctly formed.

The `edge_logits` tensor has one entry for each of the `V*(V-1)//2` edges in the complete graph on `V` vertices, where edges are each sorted and the edge order is colexicographic:

```
(0,1), (0,2), (1,2), (0,3), (1,3), (2,3), (0,4), (1,4), (2,4), ...
```

This ordering corresponds to the size-independent pairing function:

```
k = v1 + v2 * (v2 - 1) // 2
```

where `k` is the rank of the edge `(v1,v2)` in the complete graph. To convert a matrix of edge logits to the linear representation used here:

```
assert my_matrix.shape == (V, V)
i, j = make_complete_graph(V)
edge_logits = my_matrix[i, j]
```

Parameters

- **edge_logits** (*torch.Tensor*) – A tensor of length `V*(V-1)//2` containing logits (aka negative energies) of all edges in the complete graph on `V` vertices. See above comment for edge ordering.
- **sampler_options** (*dict*) – An optional dict of sampler options including: `mcmc_steps` defaulting to a single MCMC step (which is pretty good); `initial_edges` defaulting to a cheap approximate sample; `backend` one of "python" or "cpp", defaulting to "python".

arg_constraints = {'edge_logits': Real()}

enumerate_support(*expand=True*)
This is implemented for trees with up to 6 vertices (and 5 edges).

has_enumerate_support = True

log_partition_function

log_prob(*edges*)

sample(*sample_shape=torch.Size([])*)
This sampler is implemented using MCMC run for a small number of steps after being initialized by a cheap approximate sampler. This sampler is approximate and cubic time. This is faster than the classic Aldous-Broder sampler [1,2], especially for graphs with large mixing time. Recent research [3,4] proposes samplers that run in sub-matrix-multiply time but are more complex to implement.

References

[1] ***Generating random spanning trees*** Andrei Broder (1989)

[2] ***The Random Walk Construction of Uniform Spanning Trees and Uniform Labelled Trees*****,** David J. Aldous (1990)

[3] ***Sampling Random Spanning Trees Faster than Matrix Multiplication*****,** David Durfee, Rasmus Kyng, John Peebles, Anup B. Rao, Sushant Sachdeva (2017) https://arxiv.org/abs/1611.07451

[4] ***An almost-linear time algorithm for uniform random spanning tree generation*****,** Aaron Schild (2017) https://arxiv.org/abs/1711.06455

support = IntegerGreaterThan(lower_bound=0)

validate_edges(*edges*)
Validates a batch of `edges` tensors, as returned by *`sample()`* or *`enumerate_support()`* or as input to *`log_prob()`*.

Parameters **edges** (*`torch.LongTensor`*) – A batch of edges.

Raises ValueError

Returns None

4.2.38 Stable

class Stable(*stability*, *skew*, *scale=1.0*, *loc=0.0*, *coords='S0'*, *validate_args=None*)
Bases: `pyro.distributions.torch_distribution.TorchDistribution`

Levy α-stable distribution. See [1] for a review.

This uses Nolan's parametrization [2] of the `loc` parameter, which is required for continuity and differentiability. This corresponds to the notation $S^0_\alpha(\beta, \sigma, \mu_0)$ of [1], where α = stability, β = skew, σ = scale, and μ_0 = loc. To instead use the S parameterization as in scipy, pass `coords="S"`, but BEWARE this is discontinuous at `stability=1` and has poor geometry for inference.

This implements a reparametrized sampler *`rsample()`* , but does not implement *`log_prob()`* . Inference can be performed using either likelihood-free algorithms such as *`EnergyDistance`*, or reparameterization via the *`reparam()`* handler with one of the reparameterizers *`LatentStableReparam`* , *`SymmetricStableReparam`* , or *`StableReparam`* e.g.:

```
with poutine.reparam(config={"x": StableReparam()}):
    pyro.sample("x", Stable(stability, skew, scale, loc))
```

[1] S. Borak, W. Hardle, R. Weron (2005). Stable distributions. https://edoc.hu-berlin.de/bitstream/handle/18452/4526/8.pdf

[2] J.P. Nolan (1997). Numerical calculation of stable densities and distribution functions.

[3] Rafal Weron (1996). On the Chambers-Mallows-Stuck Method for Simulating Skewed Stable Random Variables.

[4] J.P. Nolan (2017). Stable Distributions: Models for Heavy Tailed Data. http://fs2.american.edu/jpnolan/www/stable/chap1.pdf

Parameters

- **stability** (*Tensor*) – Levy stability parameter $\alpha \in (0, 2]$.
- **skew** (*Tensor*) – Skewness $\beta \in [-1, 1]$.
- **scale** (*Tensor*) – Scale $\sigma > 0$. Defaults to 1.
- **loc** (*Tensor*) – Location μ_0 when using Nolan's S0 parametrization [2], or μ when using the S parameterization. Defaults to 0.
- **coords** (*str*) – Either "S0" (default) to use Nolan's continuous S0 parametrization, or "S" to use the discontinuous parameterization.

arg_constraints = {'loc': Real(), 'scale': GreaterThan(lower_bound=0.0), 'skew': In

expand(*batch_shape*, *_instance=None*)

has_rsample = True

log_prob(*value*)

mean

rsample(*sample_shape=torch.Size([])*)

support = Real()

variance

4.2.39 TruncatedPolyaGamma

class TruncatedPolyaGamma(*prototype*, *validate_args=None*)

Bases: pyro.distributions.torch_distribution.TorchDistribution

This is a PolyaGamma(1, 0) distribution truncated to have finite support in the interval (0, 2.5). See [1] for details. As a consequence of the truncation the *log_prob* method is only accurate to about six decimal places. In addition the provided sampler is a rough approximation that is only meant to be used in contexts where sample accuracy is not important (e.g. in initialization). Broadly, this implementation is only intended for usage in cases where good approximations of the *log_prob* are sufficient, as is the case e.g. in HMC.

Parameters **prototype** (*tensor*) – A prototype tensor of arbitrary shape used to determine the *dtype* and *device* returned by *sample* and *log_prob*.

References

[1] 'Bayesian inference for logistic models using Polya-Gamma latent variables' Nicholas G. Polson, James G. Scott, Jesse Windle.

arg_constraints = {}

expand(*batch_shape*, *_instance=None*)

has_rsample = False

log_prob(*value*)

num_gamma_variates = 8

num_log_prob_terms = 7

sample(*sample_shape=()*)

support = Interval(lower_bound=0.0, upper_bound=2.5)

truncation_point = 2.5

4.2.40 Unit

class Unit(*log_factor*, *validate_args=None*)

Bases: pyro.distributions.torch_distribution.TorchDistribution

Trivial nonnormalized distribution representing the unit type.

The unit type has a single value with no data, i.e. `value.numel() == 0`.

This is used for `pyro.factor()` statements.

arg_constraints = {'log_factor': Real()}

expand(*batch_shape*, *_instance=None*)

log_prob(*value*)

sample(*sample_shape=torch.Size([])*)

support = Real()

4.2.41 VonMises3D

class VonMises3D(*concentration*, *validate_args=None*)

Bases: pyro.distributions.torch_distribution.TorchDistribution

Spherical von Mises distribution.

This implementation combines the direction parameter and concentration parameter into a single combined parameter that contains both direction and magnitude. The `value` arg is represented in cartesian coordinates: it must be a normalized 3-vector that lies on the 2-sphere.

See *VonMises* for a 2D polar coordinate cousin of this distribution.

Currently only *log_prob()* is implemented.

Parameters **concentration** (*torch.Tensor*) – A combined location-and-concentration vector. The direction of this vector is the location, and its magnitude is the concentration.

arg_constraints = {'concentration': Real()}

expand(*batch_shape*)

log_prob(*value*)

support = Real()

4.2.42 ZeroInflatedDistribution

class ZeroInflatedDistribution(*base_dist*, ***, *gate=None*, *gate_logits=None*, *validate_args=None*)

Bases: pyro.distributions.torch_distribution.TorchDistribution

Generic Zero Inflated distribution.

This can be used directly or can be used as a base class as e.g. for *ZeroInflatedPoisson* and *ZeroInflatedNegativeBinomial*.

Parameters

- **base_dist** (TorchDistribution) – the base distribution.
- **gate** (*torch.Tensor*) – probability of extra zeros given via a Bernoulli distribution.
- **gate_logits** (*torch.Tensor*) – logits of extra zeros given via a Bernoulli distribution.

arg_constraints = {'gate': Interval(lower_bound=0.0, upper_bound=1.0), 'gate_logits':

expand(*batch_shape*, *_instance=None*)

gate

gate_logits

log_prob(*value*)

mean

sample(*sample_shape=torch.Size([])*)

support

variance

4.2.43 ZeroInflatedNegativeBinomial

class ZeroInflatedNegativeBinomial(*total_count*, ***, *probs=None*, *logits=None*, *gate=None*, *gate_logits=None*, *validate_args=None*)

Bases: pyro.distributions.zero_inflated.ZeroInflatedDistribution

A Zero Inflated Negative Binomial distribution.

Parameters

- **total_count** (*float or torch.Tensor*) – non-negative number of negative Bernoulli trials.
- **probs** (*torch.Tensor*) – Event probabilities of success in the half open interval [0, 1).
- **logits** (*torch.Tensor*) – Event log-odds for probabilities of success.
- **gate** (*torch.Tensor*) – probability of extra zeros.
- **gate_logits** (*torch.Tensor*) – logits of extra zeros.

arg_constraints = {'gate': Interval(lower_bound=0.0, upper_bound=1.0), 'gate_logits':

logits

probs

support = IntegerGreaterThan(lower_bound=0)

total_count

4.2.44 ZeroInflatedPoisson

class ZeroInflatedPoisson(*rate*, *, *gate=None*, *gate_logits=None*, *validate_args=None*)
Bases: pyro.distributions.zero_inflated.ZeroInflatedDistribution

A Zero Inflated Poisson distribution.

Parameters

- **rate** (*torch.Tensor*) – rate of poisson distribution.
- **gate** (*torch.Tensor*) – probability of extra zeros.
- **gate_logits** (*torch.Tensor*) – logits of extra zeros.

arg_constraints = {'gate': Interval(lower_bound=0.0, upper_bound=1.0), 'gate_logits':

rate

support = IntegerGreaterThan(lower_bound=0)

4.3 Transforms

4.3.1 ConditionalTransform

class ConditionalTransform
Bases: abc.ABC

condition(*context*)

Return type torch.distributions.Transform

4.3.2 CorrLCholeskyTransform

class CorrLCholeskyTransform(*cache_size=0*)
Bases: torch.distributions.transforms.Transform

Transforms a vector into the cholesky factor of a correlation matrix.

The input should have shape *[batch_shape] + [d * (d-1)/2]*. The output will have shape *[batch_shape] + [d, d]*.

References:

[1] Cholesky Factors of Correlation Matrices. Stan Reference Manual v2.18, Section 10.12.

bijective = True

codomain = CorrCholesky()

domain = RealVector()

event_dim = 1

log_abs_det_jacobian(*x*, *y*)

sign = 1

4.3.3 ELUTransform

class ELUTransform(*cache_size=0*)
Bases: torch.distributions.transforms.Transform

Bijective transform via the mapping $y = \text{ELU}(x)$.

bijective = True

codomain = GreaterThan(lower_bound=0.0)

domain = Real()

log_abs_det_jacobian(*x*, *y*)

sign = 1

4.3.4 HaarTransform

class HaarTransform(*dim=-1*, *flip=False*, *cache_size=0*)
Bases: torch.distributions.transforms.Transform

Discrete Haar transform.

This uses *haar_transform()* and *inverse_haar_transform()* to compute (orthonormal) Haar and inverse Haar transforms. The jacobian is 1. For sequences with length *T* not a power of two, this implementation is equivalent to a block-structured Haar transform in which block sizes decrease by factors of one half from left to right.

Parameters

- **dim** (*int*) – Dimension along which to transform. Must be negative. This is an absolute dim counting from the right.
- **flip** (*bool*) – Whether to flip the time axis before applying the Haar transform. Defaults to false.

bijective = True

codomain = RealVector()

domain = RealVector()

log_abs_det_jacobian(*x*, *y*)

with_cache(*cache_size=1*)

4.3.5 LeakyReLUTransform

class LeakyReLUTransform(*cache_size=0*)
Bases: torch.distributions.transforms.Transform

Bijective transform via the mapping $y = \text{LeakyReLU}(x)$.

bijective = True

codomain = GreaterThan(lower_bound=0.0)

domain = Real()

log_abs_det_jacobian(*x*, *y*)

sign = 1

4.3.6 LowerCholeskyAffine

class LowerCholeskyAffine(*loc*, *scale_tril*, *cache_size=0*)
Bases: torch.distributions.transforms.Transform

A bijection of the form,

$$\mathbf{y} = \mathbf{L}\mathbf{x} + \mathbf{r}$$

where *mathbf{L}* is a lower triangular matrix and *mathbf{r}* is a vector.

Parameters

- **loc** (*torch.tensor*) – the fixed D-dimensional vector to shift the input by.
- **scale_tril** (*torch.tensor*) – the D x D lower triangular matrix used in the transformation.

bijective = True

codomain = RealVector()

event_dim = 1

log_abs_det_jacobian(*x*, *y*)
Calculates the elementwise determinant of the log Jacobian, i.e. log(abs(dy/dx)).

volume_preserving = False

with_cache(*cache_size=1*)

4.3.7 OrderedTransform

class OrderedTransform(*cache_size=0*)
Bases: torch.distributions.transforms.Transform

Transforms a real vector into an ordered vector.

Specifically, enforces monotonically increasing order on the last dimension of a given tensor via the transformation $y_0 = x_0$, $y_i = \sum_{1 \leq j \leq i} \exp(x_i)$

bijective = True

codomain = OrderedVector()

domain = RealVector()

event_dim = 1

log_abs_det_jacobian(*x*, *y*)

sign = 1

4.3.8 Permute

class Permute(*permutation*, *, *dim=-1*, *cache_size=1*)
Bases: torch.distributions.transforms.Transform

A bijection that reorders the input dimensions, that is, multiplies the input by a permutation matrix. This is useful in between *AffineAutoregressive* transforms to increase the flexibility of the resulting distribution and stabilize learning. Whilst not being an autoregressive transform, the log absolute determinate of the Jacobian is easily calculable as 0. Note that reordering the input dimension between two layers of

AffineAutoregressive is not equivalent to reordering the dimension inside the MADE networks that those IAFs use; using a *Permute* transform results in a distribution with more flexibility.

Example usage:

```
>>> from pyro.nn import AutoRegressiveNN
>>> from pyro.distributions.transforms import AffineAutoregressive, Permute
>>> base_dist = dist.Normal(torch.zeros(10), torch.ones(10))
>>> iaf1 = AffineAutoregressive(AutoRegressiveNN(10, [40]))
>>> ff = Permute(torch.randperm(10, dtype=torch.long))
>>> iaf2 = AffineAutoregressive(AutoRegressiveNN(10, [40]))
>>> flow_dist = dist.TransformedDistribution(base_dist, [iaf1, ff, iaf2])
>>> flow_dist.sample()  # doctest: +SKIP
```

Parameters

- **permutation** (*torch.LongTensor*) – a permutation ordering that is applied to the inputs.
- **dim** (*int*) – the tensor dimension to permute. This value must be negative and defines the event dim as *abs(dim)*.

bijective = True

codomain = RealVector()

inv_permutation

log_abs_det_jacobian(*x*, *y*)

Calculates the elementwise determinant of the log Jacobian, i.e. log(abs([dy_0/dx_0, ..., dy_{N-1}/dx_{N-1}])). Note that this type of transform is not autoregressive, so the log Jacobian is not the sum of the previous expression. However, it turns out it's always 0 (since the determinant is -1 or +1), and so returning a vector of zeros works.

volume_preserving = True

with_cache(*cache_size=1*)

4.3.9 DiscreteCosineTransform

class DiscreteCosineTransform(*dim=-1*, *smooth=0.0*, *cache_size=0*)

Bases: torch.distributions.transforms.Transform

Discrete Cosine Transform of type-II.

This uses *dct()* and *idct()* to compute orthonormal DCT and inverse DCT transforms. The jacobian is 1.

Parameters

- **dim** (*int*) – Dimension along which to transform. Must be negative. This is an absolute dim counting from the right.
- **smooth** (*float*) – Smoothing parameter. When 0, this transforms white noise to white noise; when 1 this transforms Brownian noise to to white noise; when -1 this transforms violet noise to white noise; etc. Any real number is allowed. https://en.wikipedia.org/wiki/Colors_of_noise.

bijective = True

codomain = RealVector()

domain = RealVector()

log_abs_det_jacobian(*x*, *y*)

with_cache(*cache_size=1*)

4.4 TransformModules

4.4.1 AffineAutoregressive

class AffineAutoregressive(*autoregressive_nn*, *log_scale_min_clip=-5.0*, *log_scale_max_clip=3.0*, *sigmoid_bias=2.0*, *stable=False*)

Bases: `pyro.distributions.torch_transform.TransformModule`

An implementation of the bijective transform of Inverse Autoregressive Flow (IAF), using by default Eq (10) from Kingma Et Al., 2016,

$$\mathbf{y} = \mu_t + \sigma_t \odot \mathbf{x}$$

where $\mathbf{x}$ are the inputs, $\mathbf{y}$ are the outputs, μ_t, σ_t are calculated from an autoregressive network on $\mathbf{x}$, and $\sigma_t > 0$.

If the stable keyword argument is set to True then the transformation used is,

$$\mathbf{y} = \sigma_t \odot \mathbf{x} + (1 - \sigma_t) \odot \mu_t$$

where σ_t is restricted to $(0, 1)$. This variant of IAF is claimed by the authors to be more numerically stable than one using Eq (10), although in practice it leads to a restriction on the distributions that can be represented, presumably since the input is restricted to rescaling by a number on $(0, 1)$.

Together with *TransformedDistribution* this provides a way to create richer variational approximations.

Example usage:

```
>>> from pyro.nn import AutoRegressiveNN
>>> base_dist = dist.Normal(torch.zeros(10), torch.ones(10))
>>> transform = AffineAutoregressive(AutoRegressiveNN(10, [40]))
>>> pyro.module("my_transform", transform)  # doctest: +SKIP
>>> flow_dist = dist.TransformedDistribution(base_dist, [transform])
>>> flow_dist.sample()  # doctest: +SKIP
```

The inverse of the Bijector is required when, e.g., scoring the log density of a sample with *TransformedDistribution*. This implementation caches the inverse of the Bijector when its forward operation is called, e.g., when sampling from *TransformedDistribution*. However, if the cached value isn't available, either because it was overwritten during sampling a new value or an arbitrary value is being scored, it will calculate it manually. Note that this is an operation that scales as O(D) where D is the input dimension, and so should be avoided for large dimensional uses. So in general, it is cheap to sample from IAF and score a value that was sampled by IAF, but expensive to score an arbitrary value.

Parameters

- **autoregressive_nn** (*callable*) – an autoregressive neural network whose forward call returns a real-valued mean and logit-scale as a tuple
- **log_scale_min_clip** (*float*) – The minimum value for clipping the log(scale) from the autoregressive NN
- **log_scale_max_clip** (*float*) – The maximum value for clipping the log(scale) from the autoregressive NN

- **sigmoid_bias** (*float*) – A term to add the logit of the input when using the stable tranform.
- **stable** (*bool*) – When true, uses the alternative "stable" version of the transform (see above).

References:

[1] Diederik P. Kingma, Tim Salimans, Rafal Jozefowicz, Xi Chen, Ilya Sutskever, Max Welling. Improving Variational Inference with Inverse Autoregressive Flow. [arXiv:1606.04934]

[2] Danilo Jimenez Rezende, Shakir Mohamed. Variational Inference with Normalizing Flows. [arXiv:1505.05770]

[3] Mathieu Germain, Karol Gregor, Iain Murray, Hugo Larochelle. MADE: Masked Autoencoder for Distribution Estimation. [arXiv:1502.03509]

autoregressive = True

bijective = True

codomain = RealVector()

domain = RealVector()

event_dim = 1

log_abs_det_jacobian(*x*, *y*)
Calculates the elementwise determinant of the log Jacobian

sign = 1

4.4.2 AffineCoupling

class AffineCoupling(*split_dim*, *hypernet*, ***, *dim=-1*, *log_scale_min_clip=-5.0*, *log_scale_max_clip=3.0*)
Bases: `pyro.distributions.torch_transform.TransformModule`

An implementation of the affine coupling layer of RealNVP (Dinh et al., 2017) that uses the bijective transform,

$$\mathbf{y}_{1:d} = \mathbf{x}_{1:d} \; \mathbf{y}_{(d+1):D} = \mu + \sigma \odot \mathbf{x}_{(d+1):D}$$

where $\mathbf{x}$ are the inputs, $\mathbf{y}$ are the outputs, e.g. $\mathbf{x}_{1:d}$ represents the first d elements of the inputs, and μ, σ are shift and translation parameters calculated as the output of a function inputting only $\mathbf{x}_{1:d}$.

That is, the first d components remain unchanged, and the subsequent $D - d$ are shifted and translated by a function of the previous components.

Together with *TransformedDistribution* this provides a way to create richer variational approximations.

Example usage:

```
>>> from pyro.nn import DenseNN
>>> input_dim = 10
>>> split_dim = 6
>>> base_dist = dist.Normal(torch.zeros(input_dim), torch.ones(input_dim))
>>> param_dims = [input_dim-split_dim, input_dim-split_dim]
>>> hypernet = DenseNN(split_dim, [10*input_dim], param_dims)
>>> transform = AffineCoupling(split_dim, hypernet)
>>> pyro.module("my_transform", transform)  # doctest: +SKIP
>>> flow_dist = dist.TransformedDistribution(base_dist, [transform])
>>> flow_dist.sample()  # doctest: +SKIP
```

The inverse of the Bijector is required when, e.g., scoring the log density of a sample with *TransformedDistribution*. This implementation caches the inverse of the Bijector when its forward operation is called, e.g., when sampling from *TransformedDistribution*. However, if the cached value isn't available, either because it was overwritten during sampling a new value or an arbitary value is being scored, it will calculate it manually.

This is an operation that scales as O(1), i.e. constant in the input dimension. So in general, it is cheap to sample *and* score (an arbitrary value) from *AffineCoupling*.

Parameters

- **split_dim** (*int*) – Zero-indexed dimension d upon which to perform input/ output split for transformation.
- **hypernet** (*callable*) – a neural network whose forward call returns a real-valued mean and logit-scale as a tuple. The input should have final dimension split_dim and the output final dimension input_dim-split_dim for each member of the tuple.
- **dim** (*int*) – the tensor dimension on which to split. This value must be negative and defines the event dim as *abs(dim)*.
- **log_scale_min_clip** (*float*) – The minimum value for clipping the log(scale) from the autoregressive NN
- **log_scale_max_clip** (*float*) – The maximum value for clipping the log(scale) from the autoregressive NN

References:

[1] Laurent Dinh, Jascha Sohl-Dickstein, and Samy Bengio. Density estimation using Real NVP. ICLR 2017.

bijective = True

codomain = RealVector()

domain = RealVector()

log_abs_det_jacobian(*x*, *y*)
Calculates the elementwise determinant of the log jacobian

4.4.3 BatchNorm

class BatchNorm(*input_dim*, *momentum=0.1*, *epsilon=1e-05*)
Bases: pyro.distributions.torch_transform.TransformModule

A type of batch normalization that can be used to stabilize training in normalizing flows. The inverse operation is defined as

$$x = (y - \hat{\mu}) \oslash \sqrt{\hat{\sigma^2}} \otimes \gamma + \beta$$

that is, the standard batch norm equation, where x is the input, y is the output, γ, β are learnable parameters, and $\hat{\mu}/\hat{\sigma^2}$ are smoothed running averages of the sample mean and variance, respectively. The constraint $\gamma > 0$ is enforced to ease calculation of the log-det-Jacobian term.

This is an element-wise transform, and when applied to a vector, learns two parameters (γ, β) for each dimension of the input.

When the module is set to training mode, the moving averages of the sample mean and variance are updated every time the inverse operator is called, e.g., when a normalizing flow scores a minibatch with the *log_prob* method.

Also, when the module is set to training mode, the sample mean and variance on the current minibatch are used in place of the smoothed averages, $\hat{\mu}$ and $\hat{\sigma^2}$, for the inverse operator. For this reason it is not the case that $x = g(g^{-1}(x))$ during training, i.e., that the inverse operation is the inverse of the forward one.

Example usage:

```
>>> from pyro.nn import AutoRegressiveNN
>>> from pyro.distributions.transforms import AffineAutoregressive
>>> base_dist = dist.Normal(torch.zeros(10), torch.ones(10))
>>> iafs = [AffineAutoregressive(AutoRegressiveNN(10, [40])) for _ in range(2)]
>>> bn = BatchNorm(10)
>>> flow_dist = dist.TransformedDistribution(base_dist, [iafs[0], bn, iafs[1]])
>>> flow_dist.sample()  # doctest: +SKIP
```

Parameters

- **input_dim** (*int*) – the dimension of the input
- **momentum** (*float*) – momentum parameter for updating moving averages
- **epsilon** (*float*) – small number to add to variances to ensure numerical stability

References:

[1] Sergey Ioffe and Christian Szegedy. Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift. In International Conference on Machine Learning, 2015. https://arxiv.org/abs/1502.03167

[2] Laurent Dinh, Jascha Sohl-Dickstein, and Samy Bengio. Density Estimation using Real NVP. In International Conference on Learning Representations, 2017. https://arxiv.org/abs/1605.08803

[3] George Papamakarios, Theo Pavlakou, and Iain Murray. Masked Autoregressive Flow for Density Estimation. In Neural Information Processing Systems, 2017. https://arxiv.org/abs/1705.07057

bijective = True

codomain = Real()

constrained_gamma

domain = Real()

event_dim = 0

log_abs_det_jacobian(*x*, *y*)
Calculates the elementwise determinant of the log Jacobian, dx/dy

4.4.4 BlockAutoregressive

class BlockAutoregressive(*input_dim, hidden_factors=[8, 8], activation='tanh', residual=None*)
Bases: pyro.distributions.torch_transform.TransformModule

An implementation of Block Neural Autoregressive Flow (block-NAF) (De Cao et al., 2019) bijective transform. Block-NAF uses a similar transformation to deep dense NAF, building the autoregressive NN into the structure of the transform, in a sense.

Together with *TransformedDistribution* this provides a way to create richer variational approximations.

Example usage:

```
>>> base_dist = dist.Normal(torch.zeros(10), torch.ones(10))
>>> naf = BlockAutoregressive(input_dim=10)
>>> pyro.module("my_naf", naf)  # doctest: +SKIP
>>> naf_dist = dist.TransformedDistribution(base_dist, [naf])
>>> naf_dist.sample()  # doctest: +SKIP
```

The inverse operation is not implemented. This would require numerical inversion, e.g., using a root finding method - a possibility for a future implementation.

Parameters

- **input_dim** (*int*) – The dimensionality of the input and output variables.
- **hidden_factors** (*list*) – Hidden layer i has hidden_factors[i] hidden units per input dimension. This corresponds to both a and b in De Cao et al. (2019). The elements of hidden_factors must be integers.
- **activation** (*string*) – Activation function to use. One of 'ELU', 'LeakyReLU', 'sigmoid', or 'tanh'.
- **residual** (*string*) – Type of residual connections to use. Choices are "None", "normal" for $\mathbf{y} + f(\mathbf{y})$, and "gated" for $\alpha\mathbf{y} + (1 - \alpha\mathbf{y})$ for learnable parameter α.

References:

[1] Nicola De Cao, Ivan Titov, Wilker Aziz. Block Neural Autoregressive Flow. [arXiv:1904.04676]

autoregressive = True

bijective = True

codomain = RealVector()

domain = RealVector()

event_dim = 1

log_abs_det_jacobian(*x*, *y*)
Calculates the elementwise determinant of the log jacobian

4.4.5 ConditionalAffineAutoregressive

class ConditionalAffineAutoregressive(*autoregressive_nn*, ***kwargs*)
Bases: pyro.distributions.conditional.ConditionalTransformModule

An implementation of the bijective transform of Inverse Autoregressive Flow (IAF) that conditions on an additional context variable and uses, by default, Eq (10) from Kingma Et Al., 2016,

$$\mathbf{y} = \mu_t + \sigma_t \odot \mathbf{x}$$

where $\mathbf{x}$ are the inputs, $\mathbf{y}$ are the outputs, μ_t, σ_t are calculated from an autoregressive network on $\mathbf{x}$ and context $\mathbf{z} \in \mathbb{R}^M$, and $\sigma_t > 0$.

If the stable keyword argument is set to True then the transformation used is,

$$\mathbf{y} = \sigma_t \odot \mathbf{x} + (1 - \sigma_t) \odot \mu_t$$

where σ_t is restricted to $(0, 1)$. This variant of IAF is claimed by the authors to be more numerically stable than one using Eq (10), although in practice it leads to a restriction on the distributions that can be represented, presumably since the input is restricted to rescaling by a number on $(0, 1)$.

Together with *ConditionalTransformedDistribution* this provides a way to create richer variational approximations.

Example usage:

```
>>> from pyro.nn import ConditionalAutoRegressiveNN
>>> input_dim = 10
>>> context_dim = 4
>>> batch_size = 3
>>> hidden_dims = [10*input_dim, 10*input_dim]
>>> base_dist = dist.Normal(torch.zeros(input_dim), torch.ones(input_dim))
>>> hypernet = ConditionalAutoRegressiveNN(input_dim, context_dim, hidden_dims)
>>> transform = ConditionalAffineAutoregressive(hypernet)
>>> pyro.module("my_transform", transform)  # doctest: +SKIP
>>> z = torch.rand(batch_size, context_dim)
>>> flow_dist = dist.ConditionalTransformedDistribution(base_dist,
... [transform]).condition(z)
>>> flow_dist.sample(sample_shape=torch.Size([batch_size]))  # doctest: +SKIP
```

The inverse of the Bijector is required when, e.g., scoring the log density of a sample with *TransformedDistribution*. This implementation caches the inverse of the Bijector when its forward operation is called, e.g., when sampling from *TransformedDistribution*. However, if the cached value isn't available, either because it was overwritten during sampling a new value or an arbitrary value is being scored, it will calculate it manually. Note that this is an operation that scales as O(D) where D is the input dimension, and so should be avoided for large dimensional uses. So in general, it is cheap to sample from IAF and score a value that was sampled by IAF, but expensive to score an arbitrary value.

Parameters

- **autoregressive_nn** (*nn.Module*) – an autoregressive neural network whose forward call returns a real-valued mean and logit-scale as a tuple
- **log_scale_min_clip** (*float*) – The minimum value for clipping the log(scale) from the autoregressive NN
- **log_scale_max_clip** (*float*) – The maximum value for clipping the log(scale) from the autoregressive NN
- **sigmoid_bias** (*float*) – A term to add the logit of the input when using the stable tranform.
- **stable** (*bool*) – When true, uses the alternative "stable" version of the transform (see above).

References:

[1] Diederik P. Kingma, Tim Salimans, Rafal Jozefowicz, Xi Chen, Ilya Sutskever, Max Welling. Improving Variational Inference with Inverse Autoregressive Flow. [arXiv:1606.04934]

[2] Danilo Jimenez Rezende, Shakir Mohamed. Variational Inference with Normalizing Flows. [arXiv:1505.05770]

[3] Mathieu Germain, Karol Gregor, Iain Murray, Hugo Larochelle. MADE: Masked Autoencoder for Distribution Estimation. [arXiv:1502.03509]

bijective = True

codomain = RealVector()

condition(*context*)

Conditions on a context variable, returning a non-conditional transform of of type *AffineAutoregressive*.

domain = RealVector()

event_dim = 1

4.4.6 ConditionalAffineCoupling

class ConditionalAffineCoupling(*split_dim*, *hypernet*, ***kwargs*)
Bases: pyro.distributions.conditional.ConditionalTransformModule

An implementation of the affine coupling layer of RealNVP (Dinh et al., 2017) that conditions on an additional context variable and uses the bijective transform,

$$\mathbf{y}_{1:d} = \mathbf{x}_{1:d} \; \mathbf{y}_{(d+1):D} = \mu + \sigma \odot \mathbf{x}_{(d+1):D}$$

where $\mathbf{x}$ are the inputs, $\mathbf{y}$ are the outputs, e.g. $\mathbf{x}_{1:d}$ represents the first d elements of the inputs, and μ, σ are shift and translation parameters calculated as the output of a function input $\mathbf{x}_{1:d}$ and a context variable $\mathbf{z} \in \mathbb{R}^M$.

That is, the first d components remain unchanged, and the subsequent $D - d$ are shifted and translated by a function of the previous components.

Together with *ConditionalTransformedDistribution* this provides a way to create richer variational approximations.

Example usage:

```
>>> from pyro.nn import ConditionalDenseNN
>>> input_dim = 10
>>> split_dim = 6
>>> context_dim = 4
>>> batch_size = 3
>>> base_dist = dist.Normal(torch.zeros(input_dim), torch.ones(input_dim))
>>> param_dims = [input_dim-split_dim, input_dim-split_dim]
>>> hypernet = ConditionalDenseNN(split_dim, context_dim, [10*input_dim],
... param_dims)
>>> transform = ConditionalAffineCoupling(split_dim, hypernet)
>>> pyro.module("my_transform", transform)  # doctest: +SKIP
>>> z = torch.rand(batch_size, context_dim)
>>> flow_dist = dist.ConditionalTransformedDistribution(base_dist,
... [transform]).condition(z)
>>> flow_dist.sample(sample_shape=torch.Size([batch_size]))  # doctest: +SKIP
```

The inverse of the Bijector is required when, e.g., scoring the log density of a sample with *ConditionalTransformedDistribution*. This implementation caches the inverse of the Bijector when its forward operation is called, e.g., when sampling from *ConditionalTransformedDistribution*. However, if the cached value isn't available, either because it was overwritten during sampling a new value or an arbitary value is being scored, it will calculate it manually.

This is an operation that scales as O(1), i.e. constant in the input dimension. So in general, it is cheap to sample *and* score (an arbitrary value) from *ConditionalAffineCoupling*.

Parameters

- **split_dim** (*int*) – Zero-indexed dimension d upon which to perform input/ output split for transformation.
- **hypernet** (*callable*) – A neural network whose forward call returns a real-valued mean and logit-scale as a tuple. The input should have final dimension split_dim and the output final dimension input_dim-split_dim for each member of the tuple. The network also inputs a context variable as a keyword argument in order to condition the output upon it.
- **log_scale_min_clip** (*float*) – The minimum value for clipping the log(scale) from the NN

- **log_scale_max_clip** (*float*) – The maximum value for clipping the log(scale) from the NN

References:

Laurent Dinh, Jascha Sohl-Dickstein, and Samy Bengio. Density estimation using Real NVP. ICLR 2017.

bijective = True

codomain = RealVector()

condition(*context*)
See pyro.distributions.conditional.ConditionalTransformModule.condition()

domain = RealVector()

event_dim = 1

4.4.7 ConditionalGeneralizedChannelPermute

class ConditionalGeneralizedChannelPermute(*nn*, *channels=3*, *permutation=None*)
Bases: pyro.distributions.conditional.ConditionalTransformModule

A bijection that generalizes a permutation on the channels of a batch of 2D image in $[\ldots, C, H, W]$ format conditioning on an additional context variable. Specifically this transform performs the operation,

$$\mathbf{y} = \text{torch.nn.functional.conv2d}(\mathbf{x}, W)$$

where $\mathbf{x}$ are the inputs, $\mathbf{y}$ are the outputs, and $W \sim C \times C \times 1 \times 1$ is the filter matrix for a 1x1 convolution with C input and output channels.

Ignoring the final two dimensions, W is restricted to be the matrix product,

$$W = PLU$$

where $P \sim C \times C$ is a permutation matrix on the channel dimensions, and $LU \sim C \times C$ is an invertible product of a lower triangular and an upper triangular matrix that is the output of an NN with input $z \in \mathbb{R}^M$ representing the context variable to condition on.

The input $\mathbf{x}$ and output $\mathbf{y}$ both have shape *[...,C,H,W]*, where *C* is the number of channels set at initialization.

This operation was introduced in [1] for Glow normalizing flow, and is also known as 1x1 invertible convolution. It appears in other notable work such as [2,3], and corresponds to the class *tfp.bijectors.MatvecLU* of TensorFlow Probability.

Example usage:

```
>>> from pyro.nn.dense_nn import DenseNN
>>> context_dim = 5
>>> batch_size = 3
>>> channels = 3
>>> base_dist = dist.Normal(torch.zeros(channels, 32, 32),
... torch.ones(channels, 32, 32))
>>> hidden_dims = [context_dim*10, context_dim*10]
>>> nn = DenseNN(context_dim, hidden_dims, param_dims=[channels*channels])
>>> transform = ConditionalGeneralizedChannelPermute(nn, channels=channels)
>>> z = torch.rand(batch_size, context_dim)
>>> flow_dist = dist.ConditionalTransformedDistribution(base_dist,
... [transform]).condition(z)
>>> flow_dist.sample(sample_shape=torch.Size([batch_size])) # doctest: +SKIP
```

Parameters

- **nn** – a function inputting the context variable and outputting real-valued parameters of dimension C^2.
- **channels** (*int*) – Number of channel dimensions in the input.

[1] Diederik P. Kingma, Prafulla Dhariwal. Glow: Generative Flow with Invertible 1x1 Convolutions. [arXiv:1807.03039]

[2] Ryan Prenger, Rafael Valle, Bryan Catanzaro. WaveGlow: A Flow-based Generative Network for Speech Synthesis. [arXiv:1811.00002]

[3] Conor Durkan, Artur Bekasov, Iain Murray, George Papamakarios. Neural Spline Flows. [arXiv:1906.04032]

bijective = True

codomain = Real()

condition(*context*)
See pyro.distributions.conditional.ConditionalTransformModule.condition()

domain = Real()

event_dim = 3

4.4.8 ConditionalHouseholder

class ConditionalHouseholder(*input_dim*, *nn*, *count_transforms=1*)
Bases: pyro.distributions.conditional.ConditionalTransformModule

Represents multiple applications of the Householder bijective transformation conditioning on an additional context. A single Householder transformation takes the form,

$$\mathbf{y} = (I - 2 * \frac{\mathbf{u}\mathbf{u}^T}{||\mathbf{u}||^2})\mathbf{x}$$

where $\mathbf{x}$ are the inputs with dimension D, $\mathbf{y}$ are the outputs, and $\mathbf{u} \in \mathbb{R}^D$ is the output of a function, e.g. a NN, with input $z \in \mathbb{R}^M$ representing the context variable to condition on.

The transformation represents the reflection of $\mathbf{x}$ through the plane passing through the origin with normal $\mathbf{u}$.

D applications of this transformation are able to transform standard i.i.d. standard Gaussian noise into a Gaussian variable with an arbitrary covariance matrix. With $K < D$ transformations, one is able to approximate a full-rank Gaussian distribution using a linear transformation of rank K.

Together with *ConditionalTransformedDistribution* this provides a way to create richer variational approximations.

Example usage:

```
>>> from pyro.nn.dense_nn import DenseNN
>>> input_dim = 10
>>> context_dim = 5
>>> batch_size = 3
>>> base_dist = dist.Normal(torch.zeros(input_dim), torch.ones(input_dim))
>>> param_dims = [input_dim]
>>> hypernet = DenseNN(context_dim, [50, 50], param_dims)
>>> transform = ConditionalHouseholder(input_dim, hypernet)
>>> z = torch.rand(batch_size, context_dim)
```

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```
>>> flow_dist = dist.ConditionalTransformedDistribution(base_dist,
... [transform]).condition(z)
>>> flow_dist.sample(sample_shape=torch.Size([batch_size])) # doctest: +SKIP
```

Parameters

- **input_dim** (*int*) – the dimension of the input (and output) variable.
- **nn** (*callable*) – a function inputting the context variable and outputting a triplet of real-valued parameters of dimensions $(1, D, D)$.
- **count_transforms** (*int*) – number of applications of Householder transformation to apply.

References:

[1] Jakub M. Tomczak, Max Welling. Improving Variational Auto-Encoders using Householder Flow. [arXiv:1611.09630]

bijective = True

codomain = RealVector()

condition(*context*)

See pyro.distributions.conditional.ConditionalTransformModule.condition()

domain = RealVector()

event_dim = 1

4.4.9 ConditionalMatrixExponential

class ConditionalMatrixExponential(*input_dim*, *nn*, *iterations=8*, *normalization='none'*, *bound=None*)

Bases: pyro.distributions.conditional.ConditionalTransformModule

A dense matrix exponential bijective transform (Hoogeboom et al., 2020) that conditions on an additional context variable with equation,

$$\mathbf{y} = \exp(M)\mathbf{x}$$

where $\mathbf{x}$ are the inputs, $\mathbf{y}$ are the outputs, $\exp(\cdot)$ represents the matrix exponential, and $M \in \mathbb{R}^D \times \mathbb{R}^D$ is the output of a neural network conditioning on a context variable $\mathbf{z}$ for input dimension D. In general, M is not required to be invertible.

Due to the favourable mathematical properties of the matrix exponential, the transform has an exact inverse and a log-determinate-Jacobian that scales in time-complexity as $O(D)$. Both the forward and reverse operations are approximated with a truncated power series. For numerical stability, the norm of M can be restricted with the *normalization* keyword argument.

Example usage:

```
>>> from pyro.nn.dense_nn import DenseNN
>>> input_dim = 10
>>> context_dim = 5
>>> batch_size = 3
>>> base_dist = dist.Normal(torch.zeros(input_dim), torch.ones(input_dim))
>>> param_dims = [input_dim*input_dim]
```

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```
>>> hypernet = DenseNN(context_dim, [50, 50], param_dims)
>>> transform = ConditionalMatrixExponential(input_dim, hypernet)
>>> z = torch.rand(batch_size, context_dim)
>>> flow_dist = dist.ConditionalTransformedDistribution(base_dist,
... [transform]).condition(z)
>>> flow_dist.sample(sample_shape=torch.Size([batch_size])) # doctest: +SKIP
```

Parameters

- **input_dim** (*int*) – the dimension of the input (and output) variable.
- **iterations** (*int*) – the number of terms to use in the truncated power series that approximates matrix exponentiation.
- **normalization** (*string*) – One of *['none', 'weight', 'spectral']* normalization that selects what type of normalization to apply to the weight matrix. *weight* corresponds to weight normalization (Salimans and Kingma, 2016) and *spectral* to spectral normalization (Miyato et al, 2018).
- **bound** (*float*) – a bound on either the weight or spectral norm, when either of those two types of regularization are chosen by the *normalization* argument. A lower value for this results in fewer required terms of the truncated power series to closely approximate the exact value of the matrix exponential.

References:

[1] Emiel Hoogeboom, Victor Garcia Satorras, Jakub M. Tomczak, Max Welling. The Convolution Exponential and Generalized Sylvester Flows. [arXiv:2006.01910]

[2] Tim Salimans, Diederik P. Kingma. Weight Normalization: A Simple Reparameterization to Accelerate Training of Deep Neural Networks. [arXiv:1602.07868]

[3] Takeru Miyato, Toshiki Kataoka, Masanori Koyama, Yuichi Yoshida. Spectral Normalization for Generative Adversarial Networks. ICLR 2018.

bijective = True

codomain = RealVector()

condition(*context*)
See `pyro.distributions.conditional.ConditionalTransformModule.condition()`

domain = RealVector()

event_dim = 1

4.4.10 ConditionalNeuralAutoregressive

class ConditionalNeuralAutoregressive(*autoregressive_nn*, ***kwargs*)
Bases: `pyro.distributions.conditional.ConditionalTransformModule`

An implementation of the deep Neural Autoregressive Flow (NAF) bijective transform of the "IAF flavour" conditioning on an additiona context variable that can be used for sampling and scoring samples drawn from it (but not arbitrary ones).

Example usage:

```
>>> from pyro.nn import ConditionalAutoRegressiveNN
>>> input_dim = 10
>>> context_dim = 5
>>> batch_size = 3
>>> base_dist = dist.Normal(torch.zeros(input_dim), torch.ones(input_dim))
>>> arn = ConditionalAutoRegressiveNN(input_dim, context_dim, [40],
... param_dims=[16]*3)
>>> transform = ConditionalNeuralAutoregressive(arn, hidden_units=16)
>>> pyro.module("my_transform", transform)  # doctest: +SKIP
>>> z = torch.rand(batch_size, context_dim)
>>> flow_dist = dist.ConditionalTransformedDistribution(base_dist,
... [transform]).condition(z)
>>> flow_dist.sample(sample_shape=torch.Size([batch_size]))  # doctest: +SKIP
```

The inverse operation is not implemented. This would require numerical inversion, e.g., using a root finding method - a possibility for a future implementation.

Parameters

- **autoregressive_nn** (*nn.Module*) – an autoregressive neural network whose forward call returns a tuple of three real-valued tensors, whose last dimension is the input dimension, and whose penultimate dimension is equal to hidden_units.
- **hidden_units** (*int*) – the number of hidden units to use in the NAF transformation (see Eq (8) in reference)
- **activation** (*string*) – Activation function to use. One of 'ELU', 'LeakyReLU', 'sigmoid', or 'tanh'.

Reference:

[1] Chin-Wei Huang, David Krueger, Alexandre Lacoste, Aaron Courville. Neural Autoregressive Flows. [arXiv:1804.00779]

bijective = True

codomain = RealVector()

condition(*context*)

Conditions on a context variable, returning a non-conditional transform of of type *NeuralAutoregressive*.

domain = RealVector()

event_dim = 1

4.4.11 ConditionalPlanar

class ConditionalPlanar(*nn*)

Bases: pyro.distributions.conditional.ConditionalTransformModule

A conditional 'planar' bijective transform using the equation,

$$\mathbf{y} = \mathbf{x} + \mathbf{u}\tanh(\mathbf{w}^T\mathbf{z} + b)$$

where $\mathbf{x}$ are the inputs with dimension D, $\mathbf{y}$ are the outputs, and the pseudo-parameters $b \in \mathbb{R}$, $\mathbf{u} \in \mathbb{R}^D$, and $\mathbf{w} \in \mathbb{R}^D$ are the output of a function, e.g. a NN, with input $z \in \mathbb{R}^M$ representing the context variable to condition on. For this to be an invertible transformation, the condition $\mathbf{w}^T\mathbf{u} > -1$ is enforced.

Together with *ConditionalTransformedDistribution* this provides a way to create richer variational approximations.

Example usage:

```
>>> from pyro.nn.dense_nn import DenseNN
>>> input_dim = 10
>>> context_dim = 5
>>> batch_size = 3
>>> base_dist = dist.Normal(torch.zeros(input_dim), torch.ones(input_dim))
>>> param_dims = [1, input_dim, input_dim]
>>> hypernet = DenseNN(context_dim, [50, 50], param_dims)
>>> transform = ConditionalPlanar(hypernet)
>>> z = torch.rand(batch_size, context_dim)
>>> flow_dist = dist.ConditionalTransformedDistribution(base_dist,
... [transform]).condition(z)
>>> flow_dist.sample(sample_shape=torch.Size([batch_size])) # doctest: +SKIP
```

The inverse of this transform does not possess an analytical solution and is left unimplemented. However, the inverse is cached when the forward operation is called during sampling, and so samples drawn using the planar transform can be scored.

Parameters **nn** (*callable*) – a function inputting the context variable and outputting a triplet of real-valued parameters of dimensions $(1, D, D)$.

References: [1] Variational Inference with Normalizing Flows [arXiv:1505.05770] Danilo Jimenez Rezende, Shakir Mohamed

bijective = True

codomain = RealVector()

condition(*context*)
See pyro.distributions.conditional.ConditionalTransformModule.condition()

domain = RealVector()

event_dim = 1

4.4.12 ConditionalRadial

class ConditionalRadial(*nn*)
Bases: pyro.distributions.conditional.ConditionalTransformModule

A conditional 'radial' bijective transform context using the equation,

$$\mathbf{y} = \mathbf{x} + \beta h(\alpha, r)(\mathbf{x} - \mathbf{x}_0)$$

where $\mathbf{x}$ are the inputs, $\mathbf{y}$ are the outputs, and $\alpha \in \mathbb{R}^+$, $\beta \in \mathbb{R}$, and $\mathbf{x}_0 \in \mathbb{R}^D$, are the output of a function, e.g. a NN, with input $z \in \mathbb{R}^M$ representing the context variable to condition on. The input dimension is D, $r = ||\mathbf{x} - \mathbf{x}_0||_2$, and $h(\alpha, r) = 1/(\alpha + r)$. For this to be an invertible transformation, the condition $\beta > -\alpha$ is enforced.

Example usage:

```
>>> from pyro.nn.dense_nn import DenseNN
>>> input_dim = 10
>>> context_dim = 5
>>> batch_size = 3
>>> base_dist = dist.Normal(torch.zeros(input_dim), torch.ones(input_dim))
>>> param_dims = [input_dim, 1, 1]
>>> hypernet = DenseNN(context_dim, [50, 50], param_dims)
```

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```
>>> transform = ConditionalRadial(hypernet)
>>> z = torch.rand(batch_size, context_dim)
>>> flow_dist = dist.ConditionalTransformedDistribution(base_dist,
... [transform]).condition(z)
>>> flow_dist.sample(sample_shape=torch.Size([batch_size])) # doctest: +SKIP
```

The inverse of this transform does not possess an analytical solution and is left unimplemented. However, the inverse is cached when the forward operation is called during sampling, and so samples drawn using the radial transform can be scored.

Parameters **input_dim** (*int*) – the dimension of the input (and output) variable.

References:

[1] Danilo Jimenez Rezende, Shakir Mohamed. Variational Inference with Normalizing Flows. [arXiv:1505.05770]

bijective = True

codomain = RealVector()

condition(*context*)

See pyro.distributions.conditional.ConditionalTransformModule.condition()

domain = RealVector()

event_dim = 1

4.4.13 ConditionalSpline

class ConditionalSpline(*nn*, *input_dim*, *count_bins*, *bound=3.0*, *order='linear'*)

Bases: pyro.distributions.conditional.ConditionalTransformModule

An implementation of the element-wise rational spline bijections of linear and quadratic order (Durkan et al., 2019; Dolatabadi et al., 2020) conditioning on an additional context variable.

Rational splines are functions that are comprised of segments that are the ratio of two polynomials. For instance, for the d-th dimension and the k-th segment on the spline, the function will take the form,

$$y_d = \frac{\alpha^{(k)}(x_d)}{\beta^{(k)}(x_d)},$$

where $\alpha^{(k)}$ and $\beta^{(k)}$ are two polynomials of order d whose parameters are the output of a function, e.g. a NN, with input z
in
$mathbbR^M$ representing the context variable to condition on.. For $d = 1$, we say that the spline is linear, and for $d = 2$, quadratic. The spline is constructed on the specified bounding box, $[-K, K] \times [-K, K]$, with the identity function used elsewhere.

Rational splines offer an excellent combination of functional flexibility whilst maintaining a numerically stable inverse that is of the same computational and space complexities as the forward operation. This element-wise transform permits the accurate represention of complex univariate distributions.

Example usage:

```
>>> from pyro.nn.dense_nn import DenseNN
>>> input_dim = 10
>>> context_dim = 5
```

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```
>>> batch_size = 3
>>> count_bins = 8
>>> base_dist = dist.Normal(torch.zeros(input_dim), torch.ones(input_dim))
>>> param_dims = [input_dim * count_bins, input_dim * count_bins,
... input_dim * (count_bins - 1), input_dim * count_bins]
>>> hypernet = DenseNN(context_dim, [50, 50], param_dims)
>>> transform = ConditionalSpline(hypernet, input_dim, count_bins)
>>> z = torch.rand(batch_size, context_dim)
>>> flow_dist = dist.ConditionalTransformedDistribution(base_dist,
... [transform]).condition(z)
>>> flow_dist.sample(sample_shape=torch.Size([batch_size])) # doctest: +SKIP
```

Parameters

- **input_dim** (*int*) – Dimension of the input vector. This is required so we know how many parameters to store.
- **count_bins** (*int*) – The number of segments comprising the spline.
- **bound** (*float*) – The quantity K determining the bounding box, $[-K, K] \times [-K, K]$, of the spline.
- **order** (*string*) – One of ['linear', 'quadratic'] specifying the order of the spline.

References:

Conor Durkan, Artur Bekasov, Iain Murray, George Papamakarios. Neural Spline Flows. NeurIPS 2019.

Hadi M. Dolatabadi, Sarah Erfani, Christopher Leckie. Invertible Generative Modeling using Linear Rational Splines. AISTATS 2020.

bijective = True

codomain = Real()

condition(*context*)

See pyro.distributions.conditional.ConditionalTransformModule.condition()

domain = Real()

event_dim = 0

4.4.14 ConditionalSplineAutoregressive

class ConditionalSplineAutoregressive(*input_dim*, *autoregressive_nn*, ***kwargs*)

Bases: pyro.distributions.conditional.ConditionalTransformModule

An implementation of the autoregressive layer with rational spline bijections of linear and quadratic order (Durkan et al., 2019; Dolatabadi et al., 2020) that conditions on an additional context variable. Rational splines are functions that are comprised of segments that are the ratio of two polynomials (see *Spline*).

The autoregressive layer uses the transformation,

$$y_d = g_{\theta_d}(x_d) \quad d = 1, 2, \ldots, D$$

where $\mathbf{x} = (x_1, x_2, \ldots, x_D)$ are the inputs, $\mathbf{y} = (y_1, y_2, \ldots, y_D)$ are the outputs, g_{θ_d} is an elementwise rational monotonic spline with parameters θ_d, and $\theta = (\theta_1, \theta_2, \ldots, \theta_D)$ is the output of a conditional autoregressive NN inputting $\mathbf{x}$ and conditioning on the context variable $\mathbf{z}$.

Example usage:

```
>>> from pyro.nn import ConditionalAutoRegressiveNN
>>> input_dim = 10
>>> count_bins = 8
>>> context_dim = 5
>>> batch_size = 3
>>> base_dist = dist.Normal(torch.zeros(input_dim), torch.ones(input_dim))
>>> hidden_dims = [input_dim * 10, input_dim * 10]
>>> param_dims = [count_bins, count_bins, count_bins - 1, count_bins]
>>> hypernet = ConditionalAutoRegressiveNN(input_dim, context_dim, hidden_dims,
... param_dims=param_dims)
>>> transform = ConditionalSplineAutoregressive(input_dim, hypernet,
... count_bins=count_bins)
>>> pyro.module("my_transform", transform)  # doctest: +SKIP
>>> z = torch.rand(batch_size, context_dim)
>>> flow_dist = dist.ConditionalTransformedDistribution(base_dist,
... [transform]).condition(z)
>>> flow_dist.sample(sample_shape=torch.Size([batch_size]))  # doctest: +SKIP
```

Parameters

- **input_dim** (*int*) – Dimension of the input vector. Despite operating element-wise, this is required so we know how many parameters to store.
- **autoregressive_nn** (*callable*) – an autoregressive neural network whose forward call returns tuple of the spline parameters
- **count_bins** (*int*) – The number of segments comprising the spline.
- **bound** (*float*) – The quantity K determining the bounding box, $[-K, K] \times [-K, K]$, of the spline.
- **order** (*string*) – One of ['linear', 'quadratic'] specifying the order of the spline.

References:

Conor Durkan, Artur Bekasov, Iain Murray, George Papamakarios. Neural Spline Flows. NeurIPS 2019.

Hadi M. Dolatabadi, Sarah Erfani, Christopher Leckie. Invertible Generative Modeling using Linear Rational Splines. AISTATS 2020.

bijective = True

codomain = RealVector()

condition(*context*)
Conditions on a context variable, returning a non-conditional transform of of type *SplineAutoregressive*.

domain = RealVector()

event_dim = 1

4.4.15 ConditionalTransformModule

class ConditionalTransformModule(**args*, ***kwargs*)
Bases: pyro.distributions.conditional.ConditionalTransform, torch.nn.modules.module.Module

Conditional transforms with learnable parameters such as normalizing flows should inherit from this class rather than `ConditionalTransform` so they are also a subclass of `Module` and inherit all the useful methods of that class.

4.4.16 GeneralizedChannelPermute

class GeneralizedChannelPermute(*channels=3*, *permutation=None*)

Bases: `pyro.distributions.transforms.generalized_channel_permute.ConditionedGeneralizedChannelPermute`, `pyro.distributions.torch_transform.TransformModule`

A bijection that generalizes a permutation on the channels of a batch of 2D image in $[\ldots, C, H, W]$ format. Specifically this transform performs the operation,

$$\mathbf{y} = \text{torch.nn.functional.conv2d}(\mathbf{x}, W)$$

where $\mathbf{x}$ are the inputs, $\mathbf{y}$ are the outputs, and $W \sim C \times C \times 1 \times 1$ is the filter matrix for a 1x1 convolution with C input and output channels.

Ignoring the final two dimensions, W is restricted to be the matrix product,

$$W = PLU$$

where $P \sim C \times C$ is a permutation matrix on the channel dimensions, $L \sim C \times C$ is a lower triangular matrix with ones on the diagonal, and $U \sim C \times C$ is an upper triangular matrix. W is initialized to a random orthogonal matrix. Then, P is fixed and the learnable parameters set to L, U.

The input $\mathbf{x}$ and output $\mathbf{y}$ both have shape *[...,C,H,W]*, where *C* is the number of channels set at initialization.

This operation was introduced in [1] for Glow normalizing flow, and is also known as 1x1 invertible convolution. It appears in other notable work such as [2,3], and corresponds to the class *tfp.bijectors.MatvecLU* of TensorFlow Probability.

Example usage:

```
>>> channels = 3
>>> base_dist = dist.Normal(torch.zeros(channels, 32, 32),
... torch.ones(channels, 32, 32))
>>> inv_conv = GeneralizedChannelPermute(channels=channels)
>>> flow_dist = dist.TransformedDistribution(base_dist, [inv_conv])
>>> flow_dist.sample()  # doctest: +SKIP
```

Parameters **channels** (*int*) – Number of channel dimensions in the input.

[1] Diederik P. Kingma, Prafulla Dhariwal. Glow: Generative Flow with Invertible 1x1 Convolutions. [arXiv:1807.03039]

[2] Ryan Prenger, Rafael Valle, Bryan Catanzaro. WaveGlow: A Flow-based Generative Network for Speech Synthesis. [arXiv:1811.00002]

[3] Conor Durkan, Artur Bekasov, Iain Murray, George Papamakarios. Neural Spline Flows. [arXiv:1906.04032]

bijective = True

codomain = Real()

domain = Real()

event_dim = 3

4.4.17 Householder

class Householder(*input_dim*, *count_transforms=1*)

Bases: pyro.distributions.transforms.householder.ConditionedHouseholder, pyro.distributions.torch_transform.TransformModule

Represents multiple applications of the Householder bijective transformation. A single Householder transformation takes the form,

$$\mathbf{y} = (I - 2 * \frac{\mathbf{u}\mathbf{u}^T}{||\mathbf{u}||^2})\mathbf{x}$$

where $\mathbf{x}$ are the inputs, $\mathbf{y}$ are the outputs, and the learnable parameters are $\mathbf{u} \in \mathbb{R}^D$ for input dimension D.

The transformation represents the reflection of $\mathbf{x}$ through the plane passing through the origin with normal $\mathbf{u}$.

D applications of this transformation are able to transform standard i.i.d. standard Gaussian noise into a Gaussian variable with an arbitrary covariance matrix. With $K < D$ transformations, one is able to approximate a full-rank Gaussian distribution using a linear transformation of rank K.

Together with *TransformedDistribution* this provides a way to create richer variational approximations.

Example usage:

```
>>> base_dist = dist.Normal(torch.zeros(10), torch.ones(10))
>>> transform = Householder(10, count_transforms=5)
>>> pyro.module("my_transform", p) # doctest: +SKIP
>>> flow_dist = dist.TransformedDistribution(base_dist, [transform])
>>> flow_dist.sample()  # doctest: +SKIP
```

Parameters

- **input_dim** (*int*) – the dimension of the input (and output) variable.
- **count_transforms** (*int*) – number of applications of Householder transformation to apply.

References:

[1] Jakub M. Tomczak, Max Welling. Improving Variational Auto-Encoders using Householder Flow. [arXiv:1611.09630]

bijective = True

codomain = RealVector()

domain = RealVector()

event_dim = 1

reset_parameters()

volume_preserving = True

4.4.18 MatrixExponential

class MatrixExponential(*input_dim*, *iterations=8*, *normalization='none'*, *bound=None*)

Bases: pyro.distributions.transforms.matrix_exponential.ConditionedMatrixExponential, pyro.distributions.torch_transform.TransformModule

A dense matrix exponential bijective transform (Hoogeboom et al., 2020) with equation,

$$\mathbf{y} = \exp(M)\mathbf{x}$$

where $\mathbf{x}$ are the inputs, $\mathbf{y}$ are the outputs, $\exp(\cdot)$ represents the matrix exponential, and the learnable parameters are $M \in \mathbb{R}^D \times \mathbb{R}^D$ for input dimension D. In general, M is not required to be invertible.

Due to the favourable mathematical properties of the matrix exponential, the transform has an exact inverse and a log-determinate-Jacobian that scales in time-complexity as $O(D)$. Both the forward and reverse operations are approximated with a truncated power series. For numerical stability, the norm of M can be restricted with the *normalization* keyword argument.

Example usage:

```
>>> base_dist = dist.Normal(torch.zeros(10), torch.ones(10))
>>> transform = MatrixExponential(10)
>>> pyro.module("my_transform", transform)  # doctest: +SKIP
>>> flow_dist = dist.TransformedDistribution(base_dist, [transform])
>>> flow_dist.sample()  # doctest: +SKIP
```

Parameters

- **input_dim** (*int*) – the dimension of the input (and output) variable.
- **iterations** (*int*) – the number of terms to use in the truncated power series that approximates matrix exponentiation.
- **normalization** (*string*) – One of *['none', 'weight', 'spectral']* normalization that selects what type of normalization to apply to the weight matrix. *weight* corresponds to weight normalization (Salimans and Kingma, 2016) and *spectral* to spectral normalization (Miyato et al, 2018).
- **bound** (*float*) – a bound on either the weight or spectral norm, when either of those two types of regularization are chosen by the *normalization* argument. A lower value for this results in fewer required terms of the truncated power series to closely approximate the exact value of the matrix exponential.

References:

[1] Emiel Hoogeboom, Victor Garcia Satorras, Jakub M. Tomczak, Max Welling. The Convolution Exponential and Generalized Sylvester Flows. [arXiv:2006.01910]

[2] Tim Salimans, Diederik P. Kingma. Weight Normalization: A Simple Reparameterization to Accelerate Training of Deep Neural Networks. [arXiv:1602.07868]

[3] Takeru Miyato, Toshiki Kataoka, Masanori Koyama, Yuichi Yoshida. Spectral Normalization for Generative Adversarial Networks. ICLR 2018.

bijective = True

codomain = Real()

domain = Real()

event_dim = 1

reset_parameters()

4.4.19 NeuralAutoregressive

class NeuralAutoregressive(*autoregressive_nn*, *hidden_units=16*, *activation='sigmoid'*)

Bases: pyro.distributions.torch_transform.TransformModule

An implementation of the deep Neural Autoregressive Flow (NAF) bijective transform of the "IAF flavour" that can be used for sampling and scoring samples drawn from it (but not arbitrary ones).

Example usage:

```
>>> from pyro.nn import AutoRegressiveNN
>>> base_dist = dist.Normal(torch.zeros(10), torch.ones(10))
>>> arn = AutoRegressiveNN(10, [40], param_dims=[16]*3)
>>> transform = NeuralAutoregressive(arn, hidden_units=16)
>>> pyro.module("my_transform", transform)  # doctest: +SKIP
>>> flow_dist = dist.TransformedDistribution(base_dist, [transform])
>>> flow_dist.sample()  # doctest: +SKIP
```

The inverse operation is not implemented. This would require numerical inversion, e.g., using a root finding method - a possibility for a future implementation.

Parameters

- **autoregressive_nn** (*nn.Module*) – an autoregressive neural network whose forward call returns a tuple of three real-valued tensors, whose last dimension is the input dimension, and whose penultimate dimension is equal to hidden_units.
- **hidden_units** (*int*) – the number of hidden units to use in the NAF transformation (see Eq (8) in reference)
- **activation** (*string*) – Activation function to use. One of 'ELU', 'LeakyReLU', 'sigmoid', or 'tanh'.

Reference:

[1] Chin-Wei Huang, David Krueger, Alexandre Lacoste, Aaron Courville. Neural Autoregressive Flows. [arXiv:1804.00779]

autoregressive = True

bijective = True

codomain = RealVector()

domain = RealVector()

eps = 1e-08

event_dim = 1

log_abs_det_jacobian(*x*, *y*)
Calculates the elementwise determinant of the log Jacobian

4.4.20 Planar

class Planar(*input_dim*)
Bases: pyro.distributions.transforms.planar.ConditionedPlanar, pyro.distributions.torch_transform.TransformModule

A 'planar' bijective transform with equation,

$$\mathbf{y} = \mathbf{x} + \mathbf{u}\tanh(\mathbf{w}^T\mathbf{z} + b)$$

where $\mathbf{x}$ are the inputs, $\mathbf{y}$ are the outputs, and the learnable parameters are $b \in \mathbb{R}$, $\mathbf{u} \in \mathbb{R}^D$, $\mathbf{w} \in \mathbb{R}^D$ for input dimension D. For this to be an invertible transformation, the condition $\mathbf{w}^T\mathbf{u} > -1$ is enforced.

Together with *TransformedDistribution* this provides a way to create richer variational approximations.

Example usage:

```
>>> base_dist = dist.Normal(torch.zeros(10), torch.ones(10))
>>> transform = Planar(10)
>>> pyro.module("my_transform", transform)  # doctest: +SKIP
>>> flow_dist = dist.TransformedDistribution(base_dist, [transform])
>>> flow_dist.sample()  # doctest: +SKIP
```

The inverse of this transform does not possess an analytical solution and is left unimplemented. However, the inverse is cached when the forward operation is called during sampling, and so samples drawn using the planar transform can be scored.

Parameters **input_dim** (*int*) – the dimension of the input (and output) variable.

References:

[1] Danilo Jimenez Rezende, Shakir Mohamed. Variational Inference with Normalizing Flows. [arXiv:1505.05770]

bijective = True

codomain = RealVector()

domain = RealVector()

event_dim = 1

reset_parameters()

4.4.21 Polynomial

class Polynomial(*autoregressive_nn*, *input_dim*, *count_degree*, *count_sum*)

Bases: pyro.distributions.torch_transform.TransformModule

An autoregressive bijective transform as described in Jaini et al. (2019) applying following equation element-wise,

$$y_n = c_n + \int_0^{x_n} \sum_{k=1}^{K} \left(\sum_{r=0}^{R} a_{r,k}^{(n)} u^r \right) du$$

where x_n is the n is the n, $\left\{ a_{r,k}^{(n)} \in \mathbb{R} \right\}$ are learnable parameters that are the output of an autoregressive NN inputting $x_{\prec n} = x_1, x_2, \ldots, x_{n-1}$.

Together with *TransformedDistribution* this provides a way to create richer variational approximations.

Example usage:

```
>>> from pyro.nn import AutoRegressiveNN
>>> input_dim = 10
>>> count_degree = 4
>>> count_sum = 3
>>> base_dist = dist.Normal(torch.zeros(input_dim), torch.ones(input_dim))
>>> param_dims = [(count_degree + 1)*count_sum]
>>> arn = AutoRegressiveNN(input_dim, [input_dim*10], param_dims)
>>> transform = Polynomial(arn, input_dim=input_dim, count_degree=count_degree,
... count_sum=count_sum)
>>> pyro.module("my_transform", transform)  # doctest: +SKIP
>>> flow_dist = dist.TransformedDistribution(base_dist, [transform])
>>> flow_dist.sample()  # doctest: +SKIP
```

The inverse of this transform does not possess an analytical solution and is left unimplemented. However, the inverse is cached when the forward operation is called during sampling, and so samples drawn using a polynomial transform can be scored.

Parameters

- **autoregressive_nn** (*nn.Module*) – an autoregressive neural network whose forward call returns a tensor of real-valued numbers of size (batch_size, (count_degree+1)*count_sum, input_dim)
- **count_degree** (*int*) – The degree of the polynomial to use for each element-wise transformation.
- **count_sum** (*int*) – The number of polynomials to sum in each element-wise transformation.

References:

[1] Priyank Jaini, Kira A. Shelby, Yaoliang Yu. Sum-of-squares polynomial flow. [arXiv:1905.02325]

autoregressive = True

bijective = True

codomain = RealVector()

domain = RealVector()

event_dim = 1

log_abs_det_jacobian(*x*, *y*)
Calculates the elementwise determinant of the log Jacobian

reset_parameters()

4.4.22 Radial

class Radial(*input_dim*)
Bases: pyro.distributions.transforms.radial.ConditionedRadial, pyro.distributions.torch_transform.TransformModule

A 'radial' bijective transform using the equation,

$$\mathbf{y} = \mathbf{x} + \beta h(\alpha, r)(\mathbf{x} - \mathbf{x}_0)$$

where $\mathbf{x}$ are the inputs, $\mathbf{y}$ are the outputs, and the learnable parameters are $\alpha \in \mathbb{R}^+$, $\beta \in \mathbb{R}$, $\mathbf{x}_0 \in \mathbb{R}^D$, for input dimension D, $r = ||\mathbf{x} - \mathbf{x}_0||_2$, $h(\alpha, r) = 1/(\alpha + r)$. For this to be an invertible transformation, the condition $\beta > -\alpha$ is enforced.

Example usage:

```
>>> base_dist = dist.Normal(torch.zeros(10), torch.ones(10))
>>> transform = Radial(10)
>>> pyro.module("my_transform", transform)  # doctest: +SKIP
>>> flow_dist = dist.TransformedDistribution(base_dist, [transform])
>>> flow_dist.sample()  # doctest: +SKIP
```

The inverse of this transform does not possess an analytical solution and is left unimplemented. However, the inverse is cached when the forward operation is called during sampling, and so samples drawn using the radial transform can be scored.

Parameters **input_dim** (*int*) – the dimension of the input (and output) variable.

References:

[1] Danilo Jimenez Rezende, Shakir Mohamed. Variational Inference with Normalizing Flows. [arXiv:1505.05770]

bijective = True

codomain = RealVector()

domain = RealVector()

event_dim = 1

reset_parameters()

4.4.23 Spline

class Spline(*input_dim*, *count_bins=8*, *bound=3.0*, *order='linear'*)

Bases: pyro.distributions.transforms.spline.ConditionedSpline, pyro.distributions.torch_transform.TransformModule

An implementation of the element-wise rational spline bijections of linear and quadratic order (Durkan et al., 2019; Dolatabadi et al., 2020). Rational splines are functions that are comprised of segments that are the ratio of two polynomials. For instance, for the d-th dimension and the k-th segment on the spline, the function will take the form,

$$y_d = \frac{\alpha^{(k)}(x_d)}{\beta^{(k)}(x_d)},$$

where $\alpha^{(k)}$ and $\beta^{(k)}$ are two polynomials of order d. For $d = 1$, we say that the spline is linear, and for $d = 2$, quadratic. The spline is constructed on the specified bounding box, $[-K, K] \times [-K, K]$, with the identity function used elsewhere.

Rational splines offer an excellent combination of functional flexibility whilst maintaining a numerically stable inverse that is of the same computational and space complexities as the forward operation. This element-wise transform permits the accurate represention of complex univariate distributions.

Example usage:

```
>>> base_dist = dist.Normal(torch.zeros(10), torch.ones(10))
>>> transform = Spline(10, count_bins=4, bound=3.)
>>> pyro.module("my_transform", transform)  # doctest: +SKIP
>>> flow_dist = dist.TransformedDistribution(base_dist, [transform])
>>> flow_dist.sample()  # doctest: +SKIP
```

Parameters

- **input_dim** (*int*) – Dimension of the input vector. This is required so we know how many parameters to store.
- **count_bins** (*int*) – The number of segments comprising the spline.
- **bound** (*float*) – The quantity K determining the bounding box, $[-K, K] \times [-K, K]$, of the spline.
- **order** (*string*) – One of ['linear', 'quadratic'] specifying the order of the spline.

References:

Conor Durkan, Artur Bekasov, Iain Murray, George Papamakarios. Neural Spline Flows. NeurIPS 2019.

Hadi M. Dolatabadi, Sarah Erfani, Christopher Leckie. Invertible Generative Modeling using Linear Rational Splines. AISTATS 2020.

bijective = True

codomain = Real()

domain = Real()

event_dim = 0

4.4.24 SplineAutoregressive

class SplineAutoregressive(*input_dim*, *autoregressive_nn*, *count_bins=8*, *bound=3.0*, *order='linear'*)

Bases: pyro.distributions.torch_transform.TransformModule

An implementation of the autoregressive layer with rational spline bijections of linear and quadratic order (Durkan et al., 2019; Dolatabadi et al., 2020). Rational splines are functions that are comprised of segments that are the ratio of two polynomials (see *Spline*).

The autoregressive layer uses the transformation,

$$y_d = g_{\theta_d}(x_d) \quad d = 1, 2, \ldots, D$$

where $\mathbf{x} = (x_1, x_2, \ldots, x_D)$ are the inputs, $\mathbf{y} = (y_1, y_2, \ldots, y_D)$ are the outputs, g_{θ_d} is an elementwise rational monotonic spline with parameters θ_d, and $\theta = (\theta_1, \theta_2, \ldots, \theta_D)$ is the output of an autoregressive NN inputting $\mathbf{x}$.

Example usage:

```
>>> from pyro.nn import AutoRegressiveNN
>>> input_dim = 10
>>> count_bins = 8
>>> base_dist = dist.Normal(torch.zeros(input_dim), torch.ones(input_dim))
>>> hidden_dims = [input_dim * 10, input_dim * 10]
>>> param_dims = [count_bins, count_bins, count_bins - 1, count_bins]
>>> hypernet = AutoRegressiveNN(input_dim, hidden_dims, param_dims=param_dims)
>>> transform = SplineAutoregressive(input_dim, hypernet, count_bins=count_bins)
>>> pyro.module("my_transform", transform)  # doctest: +SKIP
>>> flow_dist = dist.TransformedDistribution(base_dist, [transform])
>>> flow_dist.sample()  # doctest: +SKIP
```

Parameters

- **input_dim** (*int*) – Dimension of the input vector. Despite operating element-wise, this is required so we know how many parameters to store.
- **autoregressive_nn** (*callable*) – an autoregressive neural network whose forward call returns tuple of the spline parameters
- **count_bins** (*int*) – The number of segments comprising the spline.
- **bound** (*float*) – The quantity K determining the bounding box, $[-K, K] \times [-K, K]$, of the spline.
- **order** (*string*) – One of ['linear', 'quadratic'] specifying the order of the spline.

References:

Conor Durkan, Artur Bekasov, Iain Murray, George Papamakarios. Neural Spline Flows. NeurIPS 2019.

Hadi M. Dolatabadi, Sarah Erfani, Christopher Leckie. Invertible Generative Modeling using Linear Rational Splines. AISTATS 2020.

autoregressive = True

bijective = True

codomain = RealVector()

domain = RealVector()

event_dim = 1

log_abs_det_jacobian(*x*, *y*)
Calculates the elementwise determinant of the log Jacobian

4.4.25 SplineCoupling

class SplineCoupling(*input_dim*, *split_dim*, *hypernet*, *count_bins=8*, *bound=3.0*, *order='linear'*, *identity=False*)
Bases: `pyro.distributions.torch_transform.TransformModule`

An implementation of the coupling layer with rational spline bijections of linear and quadratic order (Durkan et al., 2019; Dolatabadi et al., 2020). Rational splines are functions that are comprised of segments that are the ratio of two polynomials (see *Spline*).

The spline coupling layer uses the transformation,

$$\mathbf{y}_{1:d} = g_\theta(\mathbf{x}_{1:d})\ \mathbf{y}_{(d+1):D} = h_\phi(\mathbf{x}_{(d+1):D}; \mathbf{x}_{1:d})$$

where $\mathbf{x}$ are the inputs, $\mathbf{y}$ are the outputs, e.g. $\mathbf{x}_{1:d}$ represents the first d elements of the inputs, g_θ is either the identity function or an elementwise rational monotonic spline with parameters θ, and h_ϕ is a conditional elementwise spline spline, conditioning on the first d elements.

Example usage:

```
>>> from pyro.nn import DenseNN
>>> input_dim = 10
>>> split_dim = 6
>>> count_bins = 8
>>> base_dist = dist.Normal(torch.zeros(input_dim), torch.ones(input_dim))
>>> param_dims = [(input_dim - split_dim) * count_bins,
... (input_dim - split_dim) * count_bins,
... (input_dim - split_dim) * (count_bins - 1),
... (input_dim - split_dim) * count_bins]
>>> hypernet = DenseNN(split_dim, [10*input_dim], param_dims)
>>> transform = SplineCoupling(input_dim, split_dim, hypernet)
>>> pyro.module("my_transform", transform)  # doctest: +SKIP
>>> flow_dist = dist.TransformedDistribution(base_dist, [transform])
>>> flow_dist.sample()  # doctest: +SKIP
```

Parameters

- **input_dim** (*int*) – Dimension of the input vector. Despite operating element-wise, this is required so we know how many parameters to store.
- **split_dim** – Zero-indexed dimension d upon which to perform input/ output split for transformation.
- **hypernet** (*callable*) – a neural network whose forward call returns a tuple of spline parameters (see *ConditionalSpline*).

- **count_bins** (*int*) – The number of segments comprising the spline.
- **bound** (*float*) – The quantity K determining the bounding box, $[-K, K] \times [-K, K]$, of the spline.
- **order** (*string*) – One of ['linear', 'quadratic'] specifying the order of the spline.

References:

Conor Durkan, Artur Bekasov, Iain Murray, George Papamakarios. Neural Spline Flows. NeurIPS 2019.

Hadi M. Dolatabadi, Sarah Erfani, Christopher Leckie. Invertible Generative Modeling using Linear Rational Splines. AISTATS 2020.

bijective = True

codomain = RealVector()

domain = RealVector()

event_dim = 1

log_abs_det_jacobian(*x*, *y*)
Calculates the elementwise determinant of the log jacobian

4.4.26 Sylvester

class Sylvester(*input_dim*, *count_transforms=1*)
Bases: pyro.distributions.transforms.householder.Householder

An implementation of the Sylvester bijective transform of the Householder variety (Van den Berg Et Al., 2018),

$$\mathbf{y} = \mathbf{x} + QR\tanh(SQ^T\mathbf{x} + \mathbf{b})$$

where $\mathbf{x}$ are the inputs, $\mathbf{y}$ are the outputs, $R, S \sim D \times D$ are upper triangular matrices for input dimension D, $Q \sim D \times D$ is an orthogonal matrix, and $\mathbf{b} \sim D$ is learnable bias term.

The Sylvester transform is a generalization of *Planar*. In the Householder type of the Sylvester transform, the orthogonality of Q is enforced by representing it as the product of Householder transformations.

Together with *TransformedDistribution* it provides a way to create richer variational approximations.

Example usage:

```
>>> base_dist = dist.Normal(torch.zeros(10), torch.ones(10))
>>> transform = Sylvester(10, count_transforms=4)
>>> pyro.module("my_transform", transform)  # doctest: +SKIP
>>> flow_dist = dist.TransformedDistribution(base_dist, [transform])
>>> flow_dist.sample()  # doctest: +SKIP
    tensor([-0.4071, -0.5030,  0.7924, -0.2366, -0.2387, -0.1417,  0.0868,
            0.1389, -0.4629,  0.0986])
```

The inverse of this transform does not possess an analytical solution and is left unimplemented. However, the inverse is cached when the forward operation is called during sampling, and so samples drawn using the Sylvester transform can be scored.

References:

[1] Rianne van den Berg, Leonard Hasenclever, Jakub M. Tomczak, Max Welling. Sylvester Normalizing Flows for Variational Inference. UAI 2018.

Q(*x*)

R()

S()

bijective = True

codomain = RealVector()

domain = RealVector()

dtanh_dx(*x*)

event_dim = 1

log_abs_det_jacobian(*x*, *y*)
Calculates the elementwise determinant of the log Jacobian

reset_parameters2()

4.4.27 TransformModule

class TransformModule(**args*, ***kwargs*)
Bases: `torch.distributions.transforms.Transform`, `torch.nn.modules.module.Module`

Transforms with learnable parameters such as normalizing flows should inherit from this class rather than *Transform* so they are also a subclass of *nn.Module* and inherit all the useful methods of that class.

4.4.28 ComposeTransformModule

class ComposeTransformModule(*parts*)
Bases: `torch.distributions.transforms.ComposeTransform`, `torch.nn.modules.container.ModuleList`

This allows us to use a list of *TransformModule* in the same way as `ComposeTransform`. This is needed so that transform parameters are automatically registered by Pyro's param store when used in *PyroModule* instances.

4.5 Transform Factories

Each `Transform` and *TransformModule* includes a corresponding helper function in lower case that inputs, at minimum, the input dimensions of the transform, and possibly additional arguments to customize the transform in an intuitive way. The purpose of these helper functions is to hide from the user whether or not the transform requires the construction of a hypernet, and if so, the input and output dimensions of that hypernet.

4.5.1 iterated

iterated(*repeats*, *base_fn*, **args*, ***kwargs*)
Helper function to compose a sequence of bijective transforms with potentially learnable parameters using *ComposeTransformModule*.

Parameters

- **repeats** – number of repeated transforms.
- **base_fn** – function to construct the bijective transform.

- **args** – arguments taken by *base_fn*.
- **kwargs** – keyword arguments taken by *base_fn*.

Returns instance of `TransformModule`.

4.5.2 affine_autoregressive

affine_autoregressive(*input_dim*, *hidden_dims=None*, ***kwargs*)

A helper function to create an `AffineAutoregressive` object that takes care of constructing an autoregressive network with the correct input/output dimensions.

Parameters

- **input_dim** (`int`) – Dimension of input variable
- **hidden_dims** (`list[int]`) – The desired hidden dimensions of the autoregressive network. Defaults to using [3*input_dim + 1]
- **log_scale_min_clip** (`float`) – The minimum value for clipping the log(scale) from the autoregressive NN
- **log_scale_max_clip** (`float`) – The maximum value for clipping the log(scale) from the autoregressive NN
- **sigmoid_bias** (`float`) – A term to add the logit of the input when using the stable tranform.
- **stable** (`bool`) – When true, uses the alternative "stable" version of the transform (see above).

4.5.3 affine_coupling

affine_coupling(*input_dim*, *hidden_dims=None*, *split_dim=None*, *dim=-1*, ***kwargs*)

A helper function to create an `AffineCoupling` object that takes care of constructing a dense network with the correct input/output dimensions.

Parameters

- **input_dim** (`int`) – Dimension(s) of input variable to permute. Note that when *dim* < *-1* this must be a tuple corresponding to the event shape.
- **hidden_dims** (`list[int]`) – The desired hidden dimensions of the dense network. Defaults to using [10*input_dim]
- **split_dim** (`int`) – The dimension to split the input on for the coupling transform. Defaults to using input_dim // 2
- **dim** (`int`) – the tensor dimension on which to split. This value must be negative and defines the event dim as *abs(dim)*.
- **log_scale_min_clip** (`float`) – The minimum value for clipping the log(scale) from the autoregressive NN
- **log_scale_max_clip** (`float`) – The maximum value for clipping the log(scale) from the autoregressive NN

4.5.4 batchnorm

batchnorm(*input_dim*, ***kwargs*)
A helper function to create a `BatchNorm` object for consistency with other helpers.

Parameters

- **input_dim** (*int*) – Dimension of input variable
- **momentum** (*float*) – momentum parameter for updating moving averages
- **epsilon** (*float*) – small number to add to variances to ensure numerical stability

4.5.5 block_autoregressive

block_autoregressive(*input_dim*, ***kwargs*)
A helper function to create a `BlockAutoregressive` object for consistency with other helpers.

Parameters

- **input_dim** (*int*) – Dimension of input variable
- **hidden_factors** (*list*) – Hidden layer i has hidden_factors[i] hidden units per input dimension. This corresponds to both a and b in De Cao et al. (2019). The elements of hidden_factors must be integers.
- **activation** (*string*) – Activation function to use. One of 'ELU', 'LeakyReLU', 'sigmoid', or 'tanh'.
- **residual** (*string*) – Type of residual connections to use. Choices are "None", "normal" for $\mathbf{y} + f(\mathbf{y})$, and "gated" for $\alpha\mathbf{y} + (1 - \alpha\mathbf{y})$ for learnable parameter α.

4.5.6 conditional_affine_autoregressive

conditional_affine_autoregressive(*input_dim*, *context_dim*, *hidden_dims=None*, ***kwargs*)
A helper function to create an `ConditionalAffineAutoregressive` object that takes care of constructing a dense network with the correct input/output dimensions.

Parameters

- **input_dim** (*int*) – Dimension of input variable
- **context_dim** (*int*) – Dimension of context variable
- **hidden_dims** (*list[int]*) – The desired hidden dimensions of the dense network. Defaults to using [10*input_dim]
- **log_scale_min_clip** (*float*) – The minimum value for clipping the log(scale) from the autoregressive NN
- **log_scale_max_clip** (*float*) – The maximum value for clipping the log(scale) from the autoregressive NN
- **sigmoid_bias** (*float*) – A term to add the logit of the input when using the stable tranform.
- **stable** (*bool*) – When true, uses the alternative "stable" version of the transform (see above).

4.5.7 conditional_affine_coupling

conditional_affine_coupling(*input_dim*, *context_dim*, *hidden_dims=None*, *split_dim=None*, *dim=-1*, ***kwargs*)

A helper function to create an *ConditionalAffineCoupling* object that takes care of constructing a dense network with the correct input/output dimensions.

Parameters

- **input_dim** (*int*) – Dimension of input variable
- **context_dim** (*int*) – Dimension of context variable
- **hidden_dims** (*list[int]*) – The desired hidden dimensions of the dense network. Defaults to using [10*input_dim]
- **split_dim** (*int*) – The dimension to split the input on for the coupling transform. Defaults to using input_dim // 2
- **dim** (*int*) – the tensor dimension on which to split. This value must be negative and defines the event dim as *abs(dim)*.
- **log_scale_min_clip** (*float*) – The minimum value for clipping the log(scale) from the autoregressive NN
- **log_scale_max_clip** (*float*) – The maximum value for clipping the log(scale) from the autoregressive NN

4.5.8 conditional_generalized_channel_permute

conditional_generalized_channel_permute(*context_dim*, *channels=3*, *hidden_dims=None*)

A helper function to create a *ConditionalGeneralizedChannelPermute* object for consistency with other helpers.

Parameters **channels** (*int*) – Number of channel dimensions in the input.

4.5.9 conditional_householder

conditional_householder(*input_dim*, *context_dim*, *hidden_dims=None*, *count_transforms=1*)

A helper function to create a *ConditionalHouseholder* object that takes care of constructing a dense network with the correct input/output dimensions.

Parameters

- **input_dim** (*int*) – Dimension of input variable
- **context_dim** (*int*) – Dimension of context variable
- **hidden_dims** (*list[int]*) – The desired hidden dimensions of the dense network. Defaults to using [input_dim * 10, input_dim * 10]

4.5.10 conditional_matrix_exponential

conditional_matrix_exponential(*input_dim*, *context_dim*, *hidden_dims=None*, *iterations=8*, *normalization='none'*, *bound=None*)

A helper function to create a *ConditionalMatrixExponential* object for consistency with other helpers.

Parameters

- **input_dim** (*int*) – Dimension of input variable
- **context_dim** (*int*) – Dimension of context variable
- **hidden_dims** (*list[int]*) – The desired hidden dimensions of the dense network. Defaults to using [input_dim * 10, input_dim * 10]
- **iterations** (*int*) – the number of terms to use in the truncated power series that approximates matrix exponentiation.
- **normalization** (*string*) – One of *['none', 'weight', 'spectral']* normalization that selects what type of normalization to apply to the weight matrix. *weight* corresponds to weight normalization (Salimans and Kingma, 2016) and *spectral* to spectral normalization (Miyato et al, 2018).
- **bound** (*float*) – a bound on either the weight or spectral norm, when either of those two types of regularization are chosen by the *normalization* argument. A lower value for this results in fewer required terms of the truncated power series to closely approximate the exact value of the matrix exponential.

4.5.11 conditional_neural_autoregressive

conditional_neural_autoregressive(*input_dim*, *context_dim*, *hidden_dims=None*, *activation='sigmoid'*, *width=16*)

A helper function to create a *ConditionalNeuralAutoregressive* object that takes care of constructing an autoregressive network with the correct input/output dimensions.

Parameters

- **input_dim** (*int*) – Dimension of input variable
- **context_dim** (*int*) – Dimension of context variable
- **hidden_dims** (*list[int]*) – The desired hidden dimensions of the autoregressive network. Defaults to using [3*input_dim + 1]
- **activation** (*string*) – Activation function to use. One of 'ELU', 'LeakyReLU', 'sigmoid', or 'tanh'.
- **width** (*int*) – The width of the "multilayer perceptron" in the transform (see paper). Defaults to 16

4.5.12 conditional_planar

conditional_planar(*input_dim*, *context_dim*, *hidden_dims=None*)

A helper function to create a *ConditionalPlanar* object that takes care of constructing a dense network with the correct input/output dimensions.

Parameters

- **input_dim** (*int*) – Dimension of input variable
- **context_dim** (*int*) – Dimension of context variable
- **hidden_dims** (*list[int]*) – The desired hidden dimensions of the dense network. Defaults to using [input_dim * 10, input_dim * 10]

4.5.13 conditional_radial

conditional_radial(*input_dim*, *context_dim*, *hidden_dims=None*)

A helper function to create a *ConditionalRadial* object that takes care of constructing a dense network with the correct input/output dimensions.

Parameters

- **input_dim** (*int*) – Dimension of input variable
- **context_dim** (*int*) – Dimension of context variable
- **hidden_dims** (*list[int]*) – The desired hidden dimensions of the dense network. Defaults to using [input_dim * 10, input_dim * 10]

4.5.14 conditional_spline

conditional_spline(*input_dim*, *context_dim*, *hidden_dims=None*, *count_bins=8*, *bound=3.0*, *order='linear'*)

A helper function to create a *ConditionalSpline* object that takes care of constructing a dense network with the correct input/output dimensions.

Parameters

- **input_dim** (*int*) – Dimension of input variable
- **context_dim** (*int*) – Dimension of context variable
- **hidden_dims** (*list[int]*) – The desired hidden dimensions of the dense network. Defaults to using [input_dim * 10, input_dim * 10]
- **count_bins** (*int*) – The number of segments comprising the spline.
- **bound** (*float*) – The quantity K determining the bounding box, $[-K, K]imes[-K, K]$, of the spline.
- **order** (*string*) – One of ['linear', 'quadratic'] specifying the order of the spline.

4.5.15 conditional_spline_autoregressive

conditional_spline_autoregressive(*input_dim*, *context_dim*, *hidden_dims=None*, *count_bins=8*, *bound=3.0*, *order='linear'*)

A helper function to create a *ConditionalSplineAutoregressive* object that takes care of constructing an autoregressive network with the correct input/output dimensions.

Parameters

- **input_dim** (*int*) – Dimension of input variable
- **context_dim** (*int*) – Dimension of context variable
- **hidden_dims** (*list[int]*) – The desired hidden dimensions of the autoregressive network. Defaults to using [input_dim * 10, input_dim * 10]
- **count_bins** (*int*) – The number of segments comprising the spline.
- **bound** (*float*) – The quantity K determining the bounding box, $[-K, K] \times [-K, K]$, of the spline.
- **order** (*string*) – One of ['linear', 'quadratic'] specifying the order of the spline.

4.5.16 elu

elu()
A helper function to create an ELUTransform object for consistency with other helpers.

4.5.17 generalized_channel_permute

generalized_channel_permute(***kwargs*)
A helper function to create a *GeneralizedChannelPermute* object for consistency with other helpers.

Parameters **channels** (*int*) – Number of channel dimensions in the input.

4.5.18 householder

householder(*input_dim*, *count_transforms=None*)
A helper function to create a *Householder* object for consistency with other helpers.

Parameters

- **input_dim** (*int*) – Dimension of input variable
- **count_transforms** (*int*) – number of applications of Householder transformation to apply.

4.5.19 leaky_relu

leaky_relu()
A helper function to create a *LeakyReLUTransform* object for consistency with other helpers.

4.5.20 matrix_exponential

matrix_exponential(*input_dim*, *iterations=8*, *normalization='none'*, *bound=None*)
A helper function to create a *MatrixExponential* object for consistency with other helpers.

Parameters

- **input_dim** (*int*) – Dimension of input variable
- **iterations** (*int*) – the number of terms to use in the truncated power series that approximates matrix exponentiation.
- **normalization** (*string*) – One of *['none', 'weight', 'spectral']* normalization that selects what type of normalization to apply to the weight matrix. *weight* corresponds to weight normalization (Salimans and Kingma, 2016) and *spectral* to spectral normalization (Miyato et al, 2018).
- **bound** (*float*) – a bound on either the weight or spectral norm, when either of those two types of regularization are chosen by the *normalization* argument. A lower value for this results in fewer required terms of the truncated power series to closely approximate the exact value of the matrix exponential.

4.5.21 neural_autoregressive

neural_autoregressive(*input_dim*, *hidden_dims=None*, *activation='sigmoid'*, *width=16*)

A helper function to create a *NeuralAutoregressive* object that takes care of constructing an autoregressive network with the correct input/output dimensions.

Parameters

- **input_dim** (*int*) – Dimension of input variable
- **hidden_dims** (*list[int]*) – The desired hidden dimensions of the autoregressive network. Defaults to using [3*input_dim + 1]
- **activation** (*string*) – Activation function to use. One of 'ELU', 'LeakyReLU', 'sigmoid', or 'tanh'.
- **width** (*int*) – The width of the "multilayer perceptron" in the transform (see paper). Defaults to 16

4.5.22 permute

permute(*input_dim*, *permutation=None*, *dim=-1*)

A helper function to create a *Permute* object for consistency with other helpers.

Parameters

- **input_dim** (*int*) – Dimension(s) of input variable to permute. Note that when *dim < -1* this must be a tuple corresponding to the event shape.
- **permutation** (*torch.LongTensor*) – Torch tensor of integer indices representing permutation. Defaults to a random permutation.
- **dim** (*int*) – the tensor dimension to permute. This value must be negative and defines the event dim as *abs(dim)*.

4.5.23 planar

planar(*input_dim*)

A helper function to create a *Planar* object for consistency with other helpers.

Parameters **input_dim** (*int*) – Dimension of input variable

4.5.24 polynomial

polynomial(*input_dim*, *hidden_dims=None*)

A helper function to create a *Polynomial* object that takes care of constructing an autoregressive network with the correct input/output dimensions.

Parameters

- **input_dim** (*int*) – Dimension of input variable
- **hidden_dims** – The desired hidden dimensions of of the autoregressive network. Defaults to using [input_dim * 10]

4.5.25 radial

radial(*input_dim*)
A helper function to create a *Radial* object for consistency with other helpers.

Parameters **input_dim** (*int*) – Dimension of input variable

4.5.26 spline

spline(*input_dim*, ***kwargs*)
A helper function to create a *Spline* object for consistency with other helpers.

Parameters **input_dim** (*int*) – Dimension of input variable

4.5.27 spline_autoregressive

spline_autoregressive(*input_dim*, *hidden_dims=None*, *count_bins=8*, *bound=3.0*, *order='linear'*)
A helper function to create an *SplineAutoregressive* object that takes care of constructing an autoregressive network with the correct input/output dimensions.

Parameters

- **input_dim** (*int*) – Dimension of input variable
- **hidden_dims** (*list[int]*) – The desired hidden dimensions of the autoregressive network. Defaults to using [3*input_dim + 1]
- **count_bins** (*int*) – The number of segments comprising the spline.
- **bound** (*float*) – The quantity K determining the bounding box, $[-K, K] \times [-K, K]$, of the spline.
- **order** (*string*) – One of ['linear', 'quadratic'] specifying the order of the spline.

4.5.28 spline_coupling

spline_coupling(*input_dim*, *split_dim=None*, *hidden_dims=None*, *count_bins=8*, *bound=3.0*)
A helper function to create a *SplineCoupling* object for consistency with other helpers.

Parameters **input_dim** (*int*) – Dimension of input variable

4.5.29 sylvester

sylvester(*input_dim*, *count_transforms=None*)
A helper function to create a *Sylvester* object for consistency with other helpers.

Parameters

- **input_dim** (*int*) – Dimension of input variable
- **count_transforms** – Number of Sylvester operations to apply. Defaults to input_dim // 2 + 1. :type count_transforms: int

4.6 Constraints

Pyro's constraints library extends `torch.distributions.constraints`.

4.6.1 Constraint

alias of `torch.distributions.constraints.Constraint`

4.6.2 IndependentConstraint

class IndependentConstraint(*base_constraint*, *reinterpreted_batch_ndims*)

Wraps a constraint by aggregating over `reinterpreted_batch_ndims`-many dims in `check()`, so that an event is valid only if all its independent entries are valid.

Parameters

- **base_constraint** (*torch.distributions.constraints.Constraint*) – A base constraint whose entries are incidentally independent.
- **reinterpreted_batch_ndims** (*int*) – The number of extra event dimensions that will be considered dependent.

4.6.3 boolean

alias of `torch.distributions.constraints.boolean`

4.6.4 cat

alias of `torch.distributions.constraints.cat`

4.6.5 corr_cholesky_constraint

corr_cholesky_constraint

4.6.6 dependent

alias of `torch.distributions.constraints.dependent`

4.6.7 dependent_property

alias of `torch.distributions.constraints.dependent_property`

4.6.8 greater_than

alias of `torch.distributions.constraints.greater_than`

4.6.9 greater_than_eq

alias of `torch.distributions.constraints.greater_than_eq`

4.6.10 half_open_interval

alias of `torch.distributions.constraints.half_open_interval`

4.6.11 integer

`integer`

4.6.12 integer_interval

alias of `torch.distributions.constraints.integer_interval`

4.6.13 interval

alias of `torch.distributions.constraints.interval`

4.6.14 is_dependent

alias of `torch.distributions.constraints.is_dependent`

4.6.15 less_than

alias of `torch.distributions.constraints.less_than`

4.6.16 lower_cholesky

alias of `torch.distributions.constraints.lower_cholesky`

4.6.17 lower_triangular

alias of `torch.distributions.constraints.lower_triangular`

4.6.18 nonnegative_integer

alias of `torch.distributions.constraints.nonnegative_integer`

4.6.19 ordered_vector

`ordered_vector`

4.6.20 positive

alias of `torch.distributions.constraints.positive`

4.6.21 positive_definite

alias of `torch.distributions.constraints.positive_definite`

4.6.22 positive_integer

alias of `torch.distributions.constraints.positive_integer`

4.6.23 real

alias of `torch.distributions.constraints.real`

4.6.24 real_vector

alias of `torch.distributions.constraints.real_vector`

4.6.25 simplex

alias of `torch.distributions.constraints.simplex`

4.6.26 stack

alias of `torch.distributions.constraints.stack`

4.6.27 unit_interval

alias of `torch.distributions.constraints.unit_interval`

CHAPTER 5

Parameters

Parameters in Pyro are basically thin wrappers around PyTorch Tensors that carry unique names. As such Parameters are the primary stateful objects in Pyro. Users typically interact with parameters via the Pyro primitive *pyro.param*. Parameters play a central role in stochastic variational inference, where they are used to represent point estimates for the parameters in parameterized families of models and guides.

5.1 ParamStore

class ParamStoreDict

Bases: object

Global store for parameters in Pyro. This is basically a key-value store. The typical user interacts with the ParamStore primarily through the primitive *pyro.param*.

See Intro Part II for further discussion and SVI Part I for some examples.

Some things to bear in mind when using parameters in Pyro:

- parameters must be assigned unique names
- the *init_tensor* argument to *pyro.param* is only used the first time that a given (named) parameter is registered with Pyro.
- for this reason, a user may need to use the *clear()* method if working in a REPL in order to get the desired behavior. this method can also be invoked with *pyro.clear_param_store()*.
- the internal name of a parameter within a PyTorch *nn.Module* that has been registered with Pyro is prepended with the Pyro name of the module. so nothing prevents the user from having two different modules each of which contains a parameter named *weight*. by contrast, a user can only have one top-level parameter named *weight* (outside of any module).
- parameters can be saved and loaded from disk using *save* and *load*.
- in general parameters are associated with both *constrained* and *unconstrained* values. for example, under the hood a parameter that is constrained to be positive is represented as an unconstrained tensor in log space.

clear()
Clear the ParamStore

items()
Iterate over `(name, constrained_param)` pairs. Note that *constrained_param* is in the constrained (i.e. user-facing) space.

keys()
Iterate over param names.

values()
Iterate over constrained parameter values.

setdefault(*name*, *init_constrained_value*, *constraint=Real()*)
Retrieve a *constrained* parameter value from the if it exists, otherwise set the initial value. Note that this is a little fancier than `dict.setdefault()`.

If the parameter already exists, `init_constrained_tensor` will be ignored. To avoid expensive creation of `init_constrained_tensor` you can wrap it in a `lambda` that will only be evaluated if the parameter does not already exist:

```
param_store.get("foo", lambda: (0.001 * torch.randn(1000, 1000)).exp(),
                constraint=constraints.positive)
```

Parameters

- **name** (*str*) – parameter name
- **init_constrained_value** (*torch.Tensor or callable returning a torch.Tensor*) – initial constrained value
- **constraint** (*Constraint*) – torch constraint object

Returns constrained parameter value

Return type torch.Tensor

named_parameters()
Returns an iterator over `(name, unconstrained_value)` tuples for each parameter in the ParamStore. Note that, in the event the parameter is constrained, *unconstrained_value* is in the unconstrained space implicitly used by the constraint.

get_all_param_names()

replace_param(*param_name*, *new_param*, *old_param*)

get_param(*name*, *init_tensor=None*, *constraint=Real()*, *event_dim=None*)
Get parameter from its name. If it does not yet exist in the ParamStore, it will be created and stored. The Pyro primitive *pyro.param* dispatches to this method.

Parameters

- **name** (*str*) – parameter name
- **init_tensor** (*torch.Tensor*) – initial tensor
- **constraint** (*torch.distributions.constraints.Constraint*) – torch constraint
- **event_dim** (*int*) – (ignored)

Returns parameter

Return type torch.Tensor

match(*name*)
Get all parameters that match regex. The parameter must exist.

Parameters **name** (*str*) – regular expression

Returns dict with key param name and value torch Tensor

param_name(*p*)
Get parameter name from parameter

Parameters **p** – parameter

Returns parameter name

get_state()
Get the ParamStore state.

set_state(*state*)
Set the ParamStore state using state from a previous get_state() call

save(*filename*)
Save parameters to disk

Parameters **filename** (*str*) – file name to save to

load(*filename*, *map_location=None*)
Loads parameters from disk

Note: If using `pyro.module()` on parameters loaded from disk, be sure to set the `update_module_params` flag:

```
pyro.get_param_store().load('saved_params.save')
pyro.module('module', nn, update_module_params=True)
```

Parameters

- **filename** (*str*) – file name to load from
- **map_location** (*function, torch.device, string or a dict*) – specifies how to remap storage locations

param_with_module_name(*pyro_name*, *param_name*)

module_from_param_with_module_name(*param_name*)

user_param_name(*param_name*)

CHAPTER 6

Neural Networks

The module *pyro.nn* provides implementations of neural network modules that are useful in the context of deep probabilistic programming.

6.1 Pyro Modules

Pyro includes a class *PyroModule*, a subclass of `torch.nn.Module`, whose attributes can be modified by Pyro effects. To create a poutine-aware attribute, use either the *PyroParam* struct or the *PyroSample* struct:

```
my_module = PyroModule()
my_module.x = PyroParam(torch.tensor(1.), constraint=constraints.positive)
my_module.y = PyroSample(dist.Normal(0, 1))
```

class PyroParam

Bases: *pyro.nn.module.PyroParam*

Declares a Pyro-managed learnable attribute of a *PyroModule*, similar to *pyro.param*.

This can be used either to set attributes of *PyroModule* instances:

```
assert isinstance(my_module, PyroModule)
my_module.x = PyroParam(torch.zeros(4))                    # eager
my_module.y = PyroParam(lambda: torch.randn(4))            # lazy
my_module.z = PyroParam(torch.ones(4),                     # eager
                        constraint=constraints.positive,
                        event_dim=1)
```

or EXPERIMENTALLY as a decorator on lazy initialization properties:

```
class MyModule(PyroModule):
    @PyroParam
    def x(self):
        return torch.zeros(4)
```

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```
    @PyroParam
    def y(self):
        return torch.randn(4)

    @PyroParam(constraint=constraints.real, event_dim=1)
    def z(self):
        return torch.ones(4)

    def forward(self):
        return self.x + self.y + self.z  # accessed like a @property
```

Parameters

- **init_value** (*torch.Tensor or callable returning a torch.Tensor or None*) – Either a tensor for eager initialization, a callable for lazy initialization, or None for use as a decorator.
- **constraint** (*Constraint*) – torch constraint, defaults to `constraints.real`.
- **event_dim** (*int*) – (optional) number of rightmost dimensions unrelated to baching. Dimension to the left of this will be considered batch dimensions; if the param statement is inside a subsampled plate, then corresponding batch dimensions of the parameter will be correspondingly subsampled. If unspecified, all dimensions will be considered event dims and no subsampling will be performed.

class PyroSample(*prior*)

Bases: *pyro.nn.module.PyroSample*

Declares a Pyro-managed random attribute of a *PyroModule*, similar to *pyro.sample*.

This can be used either to set attributes of *PyroModule* instances:

```
assert isinstance(my_module, PyroModule)
my_module.x = PyroSample(Normal(0, 1))                    # independent
my_module.y = PyroSample(lambda self: Normal(self.x, 1))  # dependent
```

or EXPERIMENTALLY as a decorator on lazy initialization methods:

```
class MyModule(PyroModule):
    @PyroSample
    def x(self):
        return Normal(0, 1)        # independent

    @PyroSample
    def y(self):
        return Normal(self.x, 1)   # dependent

    def forward(self):
        return self.y              # accessed like a @property
```

Parameters **prior** – distribution object or function that inputs the *PyroModule* instance `self` and returns a distribution object.

class PyroModule(*name=''*)

Bases: `torch.nn.modules.module.Module`

Subclass of `torch.nn.Module` whose attributes can be modified by Pyro effects. Attributes can be set using helpers *PyroParam* and *PyroSample* , and methods can be decorated by *pyro_method()* .

Parameters

To create a Pyro-managed parameter attribute, set that attribute using either `torch.nn.Parameter` (for unconstrained parameters) or *PyroParam* (for constrained parameters). Reading that attribute will then trigger a *pyro.param* statement. For example:

```
# Create Pyro-managed parameter attributes.
my_module = PyroModule()
my_module.loc = nn.Parameter(torch.tensor(0.))
my_module.scale = PyroParam(torch.tensor(1.),
                            constraint=constraints.positive)
# Read the attributes.
loc = my_module.loc  # Triggers a pyro.param statement.
scale = my_module.scale  # Triggers another pyro.param statement.
```

Note that, unlike normal `torch.nn.Module` s, *PyroModule* s should not be registered with *pyro.module* statements. *PyroModule* s can contain other *PyroModule* s and normal `torch.nn.Module` s. Accessing a normal `torch.nn.Module` attribute of a *PyroModule* triggers a *pyro.module* statement. If multiple *PyroModule* s appear in a single Pyro model or guide, they should be included in a single root *PyroModule* for that model.

PyroModule s synchronize data with the param store at each `setattr`, `getattr`, and `delattr` event, based on the nested name of an attribute:

- Setting `mod.x = x_init` tries to read `x` from the param store. If a value is found in the param store, that value is copied into `mod` and `x_init` is ignored; otherwise `x_init` is copied into both `mod` and the param store.
- Reading `mod.x` tries to read `x` from the param store. If a value is found in the param store, that value is copied into `mod`; otherwise `mod`'s value is copied into the param store. Finally `mod` and the param store agree on a single value to return.
- Deleting `del mod.x` removes a value from both `mod` and the param store.

Note two *PyroModule* of the same name will both synchronize with the global param store and thus contain the same data. When creating a *PyroModule*, then deleting it, then creating another with the same name, the latter will be populated with the former's data from the param store. To avoid this persistence, either `pyro.clear_param_store()` or call *clear()* before deleting a *PyroModule* .

PyroModule s can be saved and loaded either directly using `torch.save()` / `torch.load()` or indirectly using the param store's *save()* / *load()* . Note that `torch.load()` will be overridden by any values in the param store, so it is safest to `pyro.clear_param_store()` before loading.

Samples

To create a Pyro-managed random attribute, set that attribute using the *PyroSample* helper, specifying a prior distribution. Reading that attribute will then trigger a *pyro.sample* statement. For example:

```
# Create Pyro-managed random attributes.
my_module.x = PyroSample(dist.Normal(0, 1))
my_module.y = PyroSample(lambda self: dist.Normal(self.loc, self.scale))

# Sample the attributes.
x = my_module.x  # Triggers a pyro.sample statement.
y = my_module.y  # Triggers one pyro.sample + two pyro.param statements.
```

Sampling is cached within each invocation of `.__call__()` or method decorated by *pyro_method()*. Because sample statements can appear only once in a Pyro trace, you should ensure that traced access to sample attributes is wrapped in a single invocation of `.__call__()` or method decorated by *pyro_method()*.

To make an existing module probabilistic, you can create a subclass and overwrite some parameters with *PyroSample* s:

```
class RandomLinear(nn.Linear, PyroModule):  # used as a mixin
    def __init__(self, in_features, out_features):
        super().__init__(in_features, out_features)
        self.weight = PyroSample(
            lambda self: dist.Normal(0, 1)
                              .expand([self.out_features,
                                       self.in_features])
                              .to_event(2))
```

Mixin classes

PyroModule can be used as a mixin class, and supports simple syntax for dynamically creating mixins, for example the following are equivalent:

```
# Version 1. create a named mixin class
class PyroLinear(nn.Linear, PyroModule):
    pass

m.linear = PyroLinear(m, n)

# Version 2. create a dynamic mixin class
m.linear = PyroModule[nn.Linear](m, n)
```

This notation can be used recursively to create Bayesian modules, e.g.:

```
model = PyroModule[nn.Sequential](
    PyroModule[nn.Linear](28 * 28, 100),
    PyroModule[nn.Sigmoid](),
    PyroModule[nn.Linear](100, 100),
    PyroModule[nn.Sigmoid](),
    PyroModule[nn.Linear](100, 10),
)
assert isinstance(model, nn.Sequential)
assert isinstance(model, PyroModule)

# Now we can be Bayesian about weights in the first layer.
model[0].weight = PyroSample(
    prior=dist.Normal(0, 1).expand([28 * 28, 100]).to_event(2))
guide = AutoDiagonalNormal(model)
```

Note that `PyroModule[...]` does not recursively mix in *PyroModule* to submodules of the input `Module`; hence we needed to wrap each submodule of the `nn.Sequential` above.

Parameters **name** (*str*) – Optional name for a root PyroModule. This is ignored in sub-PyroModules of another PyroModule.

add_module(*name*, *module*)
Adds a child module to the current module.

named_pyro_params(*prefix=''*, *recurse=True*)
Returns an iterator over PyroModule parameters, yielding both the name of the parameter as well as the parameter itself.

Parameters

- **prefix** (*str*) – prefix to prepend to all parameter names.
- **recurse** (*bool*) – if True, then yields parameters of this module and all submodules. Otherwise, yields only parameters that are direct members of this module.

Returns a generator which yields tuples containing the name and parameter

pyro_method(*fn*)

Decorator for top-level methods of a *PyroModule* to enable pyro effects and cache `pyro.sample` statements.

This should be applied to all public methods that read Pyro-managed attributes, but is not needed for `.forward()`.

clear(*mod*)

Removes data from both a *PyroModule* and the param store.

Parameters **mod** (PyroModule) – A module to clear.

to_pyro_module_(*m*, *recurse=True*)

Converts an ordinary `torch.nn.Module` instance to a *PyroModule* **in-place**.

This is useful for adding Pyro effects to third-party modules: no third-party code needs to be modified. For example:

```
model = nn.Sequential(
    nn.Linear(28 * 28, 100),
    nn.Sigmoid(),
    nn.Linear(100, 100),
    nn.Sigmoid(),
    nn.Linear(100, 10),
)
to_pyro_module_(model)
assert isinstance(model, PyroModule[nn.Sequential])
assert isinstance(model[0], PyroModule[nn.Linear])

# Now we can attempt to be fully Bayesian:
for m in model.modules():
    for name, value in list(m.named_parameters(recurse=False)):
        setattr(m, name, PyroSample(prior=dist.Normal(0, 1)
                                            .expand(value.shape)
                                            .to_event(value.dim())))
guide = AutoDiagonalNormal(model)
```

Parameters

- **m** (*torch.nn.Module*) – A module instance.
- **recurse** (*bool*) – Whether to convert submodules to `PyroModules`.

6.2 AutoRegressiveNN

class AutoRegressiveNN(*input_dim, hidden_dims, param_dims=[1, 1], permutation=None, skip_connections=False, nonlinearity=ReLU()*)

Bases: *pyro.nn.auto_reg_nn.ConditionalAutoRegressiveNN*

An implementation of a MADE-like auto-regressive neural network.

Example usage:

```
>>> x = torch.randn(100, 10)
>>> arn = AutoRegressiveNN(10, [50], param_dims=[1])
>>> p = arn(x)  # 1 parameters of size (100, 10)
>>> arn = AutoRegressiveNN(10, [50], param_dims=[1, 1])
>>> m, s = arn(x) # 2 parameters of size (100, 10)
>>> arn = AutoRegressiveNN(10, [50], param_dims=[1, 5, 3])
>>> a, b, c = arn(x) # 3 parameters of sizes, (100, 1, 10), (100, 5, 10), (100, 3,
↪ 10)
```

Parameters

- **input_dim** (*int*) – the dimensionality of the input variable
- **hidden_dims** (*list[int]*) – the dimensionality of the hidden units per layer
- **param_dims** (*list[int]*) – shape the output into parameters of dimension (p_n, input_dim) for p_n in param_dims when p_n > 1 and dimension (input_dim) when p_n == 1. The default is [1, 1], i.e. output two parameters of dimension (input_dim), which is useful for inverse autoregressive flow.
- **permutation** (*torch.LongTensor*) – an optional permutation that is applied to the inputs and controls the order of the autoregressive factorization. in particular for the identity permutation the autoregressive structure is such that the Jacobian is upper triangular. By default this is chosen at random.
- **skip_connections** (*bool*) – Whether to add skip connections from the input to the output.
- **nonlinearity** (*torch.nn.module*) – The nonlinearity to use in the feedforward network such as torch.nn.ReLU(). Note that no nonlinearity is applied to the final network output, so the output is an unbounded real number.

Reference:

MADE: Masked Autoencoder for Distribution Estimation [arXiv:1502.03509] Mathieu Germain, Karol Gregor, Iain Murray, Hugo Larochelle

forward(*x*)

6.3 DenseNN

class DenseNN(*input_dim, hidden_dims, param_dims=[1, 1], nonlinearity=ReLU()*)

Bases: *pyro.nn.dense_nn.ConditionalDenseNN*

An implementation of a simple dense feedforward network, for use in, e.g., some conditional flows such as `pyro.distributions.transforms.ConditionalPlanarFlow` and other unconditional flows such as *pyro.distributions.transforms.AffineCoupling* that do not require an autoregressive network.

Example usage:

```
>>> input_dim = 10
>>> context_dim = 5
>>> z = torch.rand(100, context_dim)
>>> nn = DenseNN(context_dim, [50], param_dims=[1, input_dim, input_dim])
>>> a, b, c = nn(z)  # parameters of size (100, 1), (100, 10), (100, 10)
```

Parameters

- **input_dim** (*int*) – the dimensionality of the input
- **hidden_dims** (*list[int]*) – the dimensionality of the hidden units per layer
- **param_dims** (*list[int]*) – shape the output into parameters of dimension (p_n,) for p_n in param_dims when p_n > 1 and dimension () when p_n == 1. The default is [1, 1], i.e. output two parameters of dimension ().
- **nonlinearity** (*torch.nn.module*) – The nonlinearity to use in the feedforward network such as torch.nn.ReLU(). Note that no nonlinearity is applied to the final network output, so the output is an unbounded real number.

forward(*x*)

6.4 ConditionalAutoRegressiveNN

class ConditionalAutoRegressiveNN(*input_dim, context_dim, hidden_dims, param_dims=[1, 1], permutation=None, skip_connections=False, nonlinearity=ReLU()*)

Bases: `torch.nn.modules.module.Module`

An implementation of a MADE-like auto-regressive neural network that can input an additional context variable. (See Reference [2] Section 3.3 for an explanation of how the conditional MADE architecture works.)

Example usage:

```
>>> x = torch.randn(100, 10)
>>> y = torch.randn(100, 5)
>>> arn = ConditionalAutoRegressiveNN(10, 5, [50], param_dims=[1])
>>> p = arn(x, context=y)  # 1 parameters of size (100, 10)
>>> arn = ConditionalAutoRegressiveNN(10, 5, [50], param_dims=[1, 1])
>>> m, s = arn(x, context=y) # 2 parameters of size (100, 10)
>>> arn = ConditionalAutoRegressiveNN(10, 5, [50], param_dims=[1, 5, 3])
>>> a, b, c = arn(x, context=y) # 3 parameters of sizes, (100, 1, 10), (100, 5,␣
↪10), (100, 3, 10)
```

Parameters

- **input_dim** (*int*) – the dimensionality of the input variable
- **context_dim** (*int*) – the dimensionality of the context variable
- **hidden_dims** (*list[int]*) – the dimensionality of the hidden units per layer
- **param_dims** (*list[int]*) – shape the output into parameters of dimension (p_n, input_dim) for p_n in param_dims when p_n > 1 and dimension (input_dim) when p_n == 1. The default is [1, 1], i.e. output two parameters of dimension (input_dim), which is useful for inverse autoregressive flow.
- **permutation** (*torch.LongTensor*) – an optional permutation that is applied to the inputs and controls the order of the autoregressive factorization. in particular for the identity permutation the autoregressive structure is such that the Jacobian is upper triangular. By default this is chosen at random.
- **skip_connections** (*bool*) – Whether to add skip connections from the input to the output.

- **nonlinearity** (*torch.nn.module*) – The nonlinearity to use in the feedforward network such as torch.nn.ReLU(). Note that no nonlinearity is applied to the final network output, so the output is an unbounded real number.

Reference:

1. MADE: Masked Autoencoder for Distribution Estimation [arXiv:1502.03509] Mathieu Germain, Karol Gregor, Iain Murray, Hugo Larochelle

2. Inference Networks for Sequential Monte Carlo in Graphical Models [arXiv:1602.06701] Brooks Paige, Frank Wood

forward(*x*, *context=None*)

get_permutation()
Get the permutation applied to the inputs (by default this is chosen at random)

6.5 ConditionalDenseNN

class ConditionalDenseNN(*input_dim, context_dim, hidden_dims, param_dims=[1, 1], nonlinearity=ReLU()*)
Bases: `torch.nn.modules.module.Module`

An implementation of a simple dense feedforward network taking a context variable, for use in, e.g., some conditional flows such as *pyro.distributions.transforms.ConditionalAffineCoupling*.

Example usage:

```
>>> input_dim = 10
>>> context_dim = 5
>>> x = torch.rand(100, input_dim)
>>> z = torch.rand(100, context_dim)
>>> nn = ConditionalDenseNN(input_dim, context_dim, [50], param_dims=[1, input_
↪dim, input_dim])
>>> a, b, c = nn(x, context=z)  # parameters of size (100, 1), (100, 10), (100,␣
↪10)
```

Parameters

- **input_dim** (*int*) – the dimensionality of the input
- **context_dim** (*int*) – the dimensionality of the context variable
- **hidden_dims** (*list[int]*) – the dimensionality of the hidden units per layer
- **param_dims** (*list[int]*) – shape the output into parameters of dimension (p_n,) for p_n in param_dims when p_n > 1 and dimension () when p_n == 1. The default is [1, 1], i.e. output two parameters of dimension ().
- **nonlinearity** (*torch.nn.Module*) – The nonlinearity to use in the feedforward network such as torch.nn.ReLU(). Note that no nonlinearity is applied to the final network output, so the output is an unbounded real number.

forward(*x*, *context*)

CHAPTER 7

Optimization

The module *pyro.optim* provides support for optimization in Pyro. In particular it provides *PyroOptim*, which is used to wrap PyTorch optimizers and manage optimizers for dynamically generated parameters (see the tutorial SVI Part I for a discussion). Any custom optimization algorithms are also to be found here.

7.1 Pyro Optimizers

class PyroOptim(*optim_constructor*, *optim_args*, *clip_args=None*)

Bases: `object`

A wrapper for torch.optim.Optimizer objects that helps with managing dynamically generated parameters.

Parameters

- **optim_constructor** – a torch.optim.Optimizer
- **optim_args** – a dictionary of learning arguments for the optimizer or a callable that returns such dictionaries
- **clip_args** – a dictionary of clip_norm and/or clip_value args or a callable that returns such dictionaries

__call__(*params*, **args*, ***kwargs*)

Parameters **params** (*an iterable of strings*) – a list of parameters

Do an optimization step for each param in params. If a given param has never been seen before, initialize an optimizer for it.

get_state()

Get state associated with all the optimizers in the form of a dictionary with key-value pairs (parameter name, optim state dicts)

set_state(*state_dict*)

Set the state associated with all the optimizers using the state obtained from a previous call to get_state()

save(*filename*)

Parameters **filename** (*str*) – file name to save to

Save optimizer state to disk

load(*filename*)

Parameters **filename** (*str*) – file name to load from

Load optimizer state from disk

AdagradRMSProp(*optim_args*)
Wraps *pyro.optim.adagrad_rmsprop.AdagradRMSProp* with *PyroOptim*.

ClippedAdam(*optim_args*)
Wraps *pyro.optim.clipped_adam.ClippedAdam* with *PyroOptim*.

DCTAdam(*optim_args*)
Wraps `pyro.optim.dct_adam.DCTAdam` with *PyroOptim*.

class PyroLRScheduler(*scheduler_constructor*, *optim_args*, *clip_args=None*)
Bases: *pyro.optim.optim.PyroOptim*

A wrapper for `lr_scheduler` objects that adjusts learning rates for dynamically generated parameters.

Parameters

- **scheduler_constructor** – a `lr_scheduler`
- **optim_args** – a dictionary of learning arguments for the optimizer or a callable that returns such dictionaries. must contain the key 'optimizer' with pytorch optimizer value
- **clip_args** – a dictionary of clip_norm and/or clip_value args or a callable that returns such dictionaries.

Example:

```
optimizer = torch.optim.SGD
scheduler = pyro.optim.ExponentialLR({'optimizer': optimizer, 'optim_args': {'lr
↪': 0.01}, 'gamma': 0.1})
svi = SVI(model, guide, scheduler, loss=TraceGraph_ELBO())
for i in range(epochs):
    for minibatch in DataLoader(dataset, batch_size):
        svi.step(minibatch)
    scheduler.step()
```

__call__(*params*, **args*, ***kwargs*)

step(**args*, ***kwargs*)
Takes the same arguments as the PyTorch scheduler (e.g. optional `loss` for `ReduceLROnPlateau`)

class AdagradRMSProp(*params*, *eta=1.0*, *delta=1e-16*, *t=0.1*)
Bases: `torch.optim.optimizer.Optimizer`

Implements a mash-up of the Adagrad algorithm and RMSProp. For the precise update equation see equations 10 and 11 in reference [1].

References: [1] 'Automatic Differentiation Variational Inference', Alp Kucukelbir, Dustin Tran, Rajesh Ranganath, Andrew Gelman, David M. Blei URL: https://arxiv.org/abs/1603.00788 [2] 'Lecture 6.5 RmsProp: Divide the gradient by a running average of its recent magnitude', Tieleman, T. and Hinton, G., COURSERA: Neural Networks for Machine Learning. [3] 'Adaptive subgradient methods for online learning and stochastic optimization', Duchi, John, Hazan, E and Singer, Y.

Arguments:

Parameters

- **params** – iterable of parameters to optimize or dicts defining parameter groups
- **eta** (*float*) – sets the step size scale (optional; default: 1.0)
- **t** (*float*) – t, optional): momentum parameter (optional; default: 0.1)
- **delta** (*float*) – modulates the exponent that controls how the step size scales (optional: default: 1e-16)

share_memory()

step(*closure=None*)

Performs a single optimization step.

Parameters **closure** – A (optional) closure that reevaluates the model and returns the loss.

class ClippedAdam(*params*, *lr=0.001*, *betas=(0.9*, *0.999)*, *eps=1e-08*, *weight_decay=0*, *clip_norm=10.0*, *lrd=1.0*)

Bases: torch.optim.optimizer.Optimizer

Parameters

- **params** – iterable of parameters to optimize or dicts defining parameter groups
- **lr** – learning rate (default: 1e-3)
- **betas** (*Tuple*) – coefficients used for computing running averages of gradient and its square (default: (0.9, 0.999))
- **eps** – term added to the denominator to improve numerical stability (default: 1e-8)
- **weight_decay** – weight decay (L2 penalty) (default: 0)
- **clip_norm** – magnitude of norm to which gradients are clipped (default: 10.0)
- **lrd** – rate at which learning rate decays (default: 1.0)

Small modification to the Adam algorithm implemented in torch.optim.Adam to include gradient clipping and learning rate decay.

Reference

A Method for Stochastic Optimization, Diederik P. Kingma, Jimmy Ba https://arxiv.org/abs/1412.6980

step(*closure=None*)

Parameters **closure** – An optional closure that reevaluates the model and returns the loss.

Performs a single optimization step.

class HorovodOptimizer(*pyro_optim*, ***horovod_kwargs*)

Bases: *pyro.optim.optim.PyroOptim*

Distributed wrapper for a *PyroOptim* optimizer.

This class wraps a PyroOptim object similar to the way horovod.torch.DistributedOptimizer() wraps a torch.optim.Optimizer.

Note: This requires horovod.torch to be installed, e.g. via pip install pyro[horovod]. For details see https://horovod.readthedocs.io/en/stable/install.html

---

Param A Pyro optimizer instance.

Parameters ****horovod_kwargs** – Extra parameters passed to horovod.torch.DistributedOptimizer().

__call__(*params*, **args*, ***kwargs*)

7.2 PyTorch Optimizers

Adadelta(*optim_args*, *clip_args=None*)
Wraps `torch.optim.Adadelta` with *PyroOptim*.

Adagrad(*optim_args*, *clip_args=None*)
Wraps `torch.optim.Adagrad` with *PyroOptim*.

Adam(*optim_args*, *clip_args=None*)
Wraps `torch.optim.Adam` with *PyroOptim*.

AdamW(*optim_args*, *clip_args=None*)
Wraps `torch.optim.AdamW` with *PyroOptim*.

SparseAdam(*optim_args*, *clip_args=None*)
Wraps `torch.optim.SparseAdam` with *PyroOptim*.

Adamax(*optim_args*, *clip_args=None*)
Wraps `torch.optim.Adamax` with *PyroOptim*.

ASGD(*optim_args*, *clip_args=None*)
Wraps `torch.optim.ASGD` with *PyroOptim*.

SGD(*optim_args*, *clip_args=None*)
Wraps `torch.optim.SGD` with *PyroOptim*.

Rprop(*optim_args*, *clip_args=None*)
Wraps `torch.optim.Rprop` with *PyroOptim*.

RMSprop(*optim_args*, *clip_args=None*)
Wraps `torch.optim.RMSprop` with *PyroOptim*.

LambdaLR(*optim_args*, *clip_args=None*)
Wraps `torch.optim.LambdaLR` with *PyroLRScheduler*.

MultiplicativeLR(*optim_args*, *clip_args=None*)
Wraps `torch.optim.MultiplicativeLR` with *PyroLRScheduler*.

StepLR(*optim_args*, *clip_args=None*)
Wraps `torch.optim.StepLR` with *PyroLRScheduler*.

MultiStepLR(*optim_args*, *clip_args=None*)
Wraps `torch.optim.MultiStepLR` with *PyroLRScheduler*.

ExponentialLR(*optim_args*, *clip_args=None*)
Wraps `torch.optim.ExponentialLR` with *PyroLRScheduler*.

CosineAnnealingLR(*optim_args*, *clip_args=None*)
Wraps `torch.optim.CosineAnnealingLR` with *PyroLRScheduler*.

ReduceLROnPlateau(*optim_args*, *clip_args=None*)
Wraps `torch.optim.ReduceLROnPlateau` with *PyroLRScheduler*.

CyclicLR(*optim_args*, *clip_args=None*)
Wraps `torch.optim.CyclicLR` with *PyroLRScheduler*.

CosineAnnealingWarmRestarts(*optim_args*, *clip_args=None*)
Wraps `torch.optim.CosineAnnealingWarmRestarts` with *PyroLRScheduler*.

OneCycleLR(*optim_args*, *clip_args=None*)
Wraps `torch.optim.OneCycleLR` with *PyroLRScheduler*.

7.3 Higher-Order Optimizers

class MultiOptimizer
Bases: `object`

Base class of optimizers that make use of higher-order derivatives.

Higher-order optimizers generally use `torch.autograd.grad()` rather than `torch.Tensor.backward()`, and therefore require a different interface from usual Pyro and PyTorch optimizers. In this interface, the *step()* method inputs a `loss` tensor to be differentiated, and backpropagation is triggered one or more times inside the optimizer.

Derived classes must implement *step()* to compute derivatives and update parameters in-place.

Example:

```
tr = poutine.trace(model).get_trace(*args, **kwargs)
loss = -tr.log_prob_sum()
params = {name: site['value'].unconstrained()
          for name, site in tr.nodes.items()
          if site['type'] == 'param'}
optim.step(loss, params)
```

step(*loss*, *params*)
Performs an in-place optimization step on parameters given a differentiable `loss` tensor.

Note that this detaches the updated tensors.

Parameters

- **loss** (*torch.Tensor*) – A differentiable tensor to be minimized. Some optimizers require this to be differentiable multiple times.
- **params** (*dict*) – A dictionary mapping param name to unconstrained value as stored in the param store.

get_step(*loss*, *params*)
Computes an optimization step of parameters given a differentiable `loss` tensor, returning the updated values.

Note that this preserves derivatives on the updated tensors.

Parameters

- **loss** (*torch.Tensor*) – A differentiable tensor to be minimized. Some optimizers require this to be differentiable multiple times.
- **params** (*dict*) – A dictionary mapping param name to unconstrained value as stored in the param store.

Returns A dictionary mapping param name to updated unconstrained value.

Return type dict

class PyroMultiOptimizer(*optim*)
Bases: *pyro.optim.multi.MultiOptimizer*

Facade to wrap *PyroOptim* objects in a *MultiOptimizer* interface.

step(*loss*, *params*)

class TorchMultiOptimizer(*optim_constructor*, *optim_args*)
Bases: *pyro.optim.multi.PyroMultiOptimizer*

Facade to wrap `Optimizer` objects in a *MultiOptimizer* interface.

class MixedMultiOptimizer(*parts*)
Bases: *pyro.optim.multi.MultiOptimizer*

Container class to combine different *MultiOptimizer* instances for different parameters.

Parameters **parts** (*list*) – A list of `(names, optim)` pairs, where each `names` is a list of parameter names, and each `optim` is a *MultiOptimizer* or *PyroOptim* object to be used for the named parameters. Together the `names` should partition up all desired parameters to optimize.

Raises **ValueError** – if any name is optimized by multiple optimizers.

step(*loss*, *params*)

get_step(*loss*, *params*)

class Newton(*trust_radii={}*)
Bases: *pyro.optim.multi.MultiOptimizer*

Implementation of *MultiOptimizer* that performs a Newton update on batched low-dimensional variables, optionally regularizing via a per-parameter `trust_radius`. See *newton_step()* for details.

The result of *get_step()* will be differentiable, however the updated values from `step()` will be detached.

Parameters **trust_radii** (*dict*) – a dict mapping parameter name to radius of trust region. Missing names will use unregularized Newton update, equivalent to infinite trust radius.

get_step(*loss*, *params*)

CHAPTER 8

Poutine (Effect handlers)

Beneath the built-in inference algorithms, Pyro has a library of composable effect handlers for creating new inference algorithms and working with probabilistic programs. Pyro's inference algorithms are all built by applying these handlers to stochastic functions.

8.1 Handlers

Poutine is a library of composable effect handlers for recording and modifying the behavior of Pyro programs. These lower-level ingredients simplify the implementation of new inference algorithms and behavior.

Handlers can be used as higher-order functions, decorators, or context managers to modify the behavior of functions or blocks of code:

For example, consider the following Pyro program:

```
>>> def model(x):
...     s = pyro.param("s", torch.tensor(0.5))
...     z = pyro.sample("z", dist.Normal(x, s))
...     return z ** 2
```

We can mark sample sites as observed using `condition`, which returns a callable with the same input and output signatures as `model`:

```
>>> conditioned_model = poutine.condition(model, data={"z": 1.0})
```

We can also use handlers as decorators:

```
>>> @pyro.condition(data={"z": 1.0})
... def model(x):
...     s = pyro.param("s", torch.tensor(0.5))
...     z = pyro.sample("z", dist.Normal(x, s))
...     return z ** 2
```

Or as context managers:

```
>>> with pyro.condition(data={"z": 1.0}):
...     s = pyro.param("s", torch.tensor(0.5))
...     z = pyro.sample("z", dist.Normal(0., s))
...     y = z ** 2
```

Handlers compose freely:

```
>>> conditioned_model = poutine.condition(model, data={"z": 1.0})
>>> traced_model = poutine.trace(conditioned_model)
```

Many inference algorithms or algorithmic components can be implemented in just a few lines of code:

```
guide_tr = poutine.trace(guide).get_trace(...)
model_tr = poutine.trace(poutine.replay(conditioned_model, trace=guide_tr)).get_
↪trace(...)
monte_carlo_elbo = model_tr.log_prob_sum() - guide_tr.log_prob_sum()
```

block (*fn=None*, **args*, ***kwargs*)

Convenient wrapper of *BlockMessenger*

This handler selectively hides Pyro primitive sites from the outside world. Default behavior: block everything.

A site is hidden if at least one of the following holds:

0. `hide_fn(msg) is True` or `(not expose_fn(msg)) is True`
1. `msg["name"] in hide`
2. `msg["type"] in hide_types`
3. `msg["name"] not in expose and msg["type"] not in expose_types`
4. `hide`, `hide_types`, and `expose_types` are all `None`

For example, suppose the stochastic function fn has two sample sites "a" and "b". Then any effect outside of `BlockMessenger(fn, hide=["a"])` will not be applied to site "a" and will only see site "b":

```
>>> def fn():
...     a = pyro.sample("a", dist.Normal(0., 1.))
...     return pyro.sample("b", dist.Normal(a, 1.))
>>> fn_inner = pyro.poutine.trace(fn)
>>> fn_outer = pyro.poutine.trace(pyro.poutine.block(fn_inner, hide=["a"]))
>>> trace_inner = fn_inner.get_trace()
>>> trace_outer  = fn_outer.get_trace()
>>> "a" in trace_inner
True
>>> "a" in trace_outer
False
>>> "b" in trace_inner
True
>>> "b" in trace_outer
True
```

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls)
- **hide_fn** – function that takes a site and returns True to hide the site or False/None to expose it. If specified, all other parameters are ignored. Only specify one of hide_fn or expose_fn, not both.

- **expose_fn** – function that takes a site and returns True to expose the site or False/None to hide it. If specified, all other parameters are ignored. Only specify one of hide_fn or expose_fn, not both.
- **hide_all** (*bool*) – hide all sites
- **expose_all** (*bool*) – expose all sites normally
- **hide** (*list*) – list of site names to hide
- **expose** (*list*) – list of site names to be exposed while all others hidden
- **hide_types** (*list*) – list of site types to be hidden
- **expose_types** (*lits*) – list of site types to be exposed while all others hidden

Returns stochastic function decorated with a *BlockMessenger*

broadcast (*fn=None*, **args*, ***kwargs*)
Convenient wrapper of *BroadcastMessenger*

Automatically broadcasts the batch shape of the stochastic function at a sample site when inside a single or nested plate context. The existing *batch_shape* must be broadcastable with the size of the `plate` contexts installed in the *cond_indep_stack*.

Notice how *model_automatic_broadcast* below automates expanding of distribution batch shapes. This makes it easy to modularize a Pyro model as the sub-components are agnostic of the wrapping `plate` contexts.

```
>>> def model_broadcast_by_hand():
...     with IndepMessenger("batch", 100, dim=-2):
...         with IndepMessenger("components", 3, dim=-1):
...             sample = pyro.sample("sample", dist.Bernoulli(torch.ones(3) * 0.5)
...                                                 .expand_by(100))
...             assert sample.shape == torch.Size((100, 3))
...     return sample
```

```
>>> @poutine.broadcast
... def model_automatic_broadcast():
...     with IndepMessenger("batch", 100, dim=-2):
...         with IndepMessenger("components", 3, dim=-1):
...             sample = pyro.sample("sample", dist.Bernoulli(torch.tensor(0.5)))
...             assert sample.shape == torch.Size((100, 3))
...     return sample
```

collapse (*fn=None*, **args*, ***kwargs*)
Convenient wrapper of *CollapseMessenger*

EXPERIMENTAL Collapses all sites in the context by lazily sampling and attempting to use conjugacy relations. If no conjugacy is known this will fail. Code using the results of sample sites must be written to accept Funsors rather than Tensors. This requires `funsor` to be installed.

> **Warning:** This is not compatible with automatic guessing of `max_plate_nesting`. If any plates appear within the collapsed context, you should manually declare `max_plate_nesting` to your inference algorithm (e.g. `Trace_ELBO(max_plate_nesting=1)`).

condition (*fn=None*, **args*, ***kwargs*)
Convenient wrapper of *ConditionMessenger*

Given a stochastic function with some sample statements and a dictionary of observations at names, change the sample statements at those names into observes with those values.

Consider the following Pyro program:

```
>>> def model(x):
...     s = pyro.param("s", torch.tensor(0.5))
...     z = pyro.sample("z", dist.Normal(x, s))
...     return z ** 2
```

To observe a value for site *z*, we can write

```
>>> conditioned_model = pyro.poutine.condition(model, data={"z": torch.tensor(1.)}
↪)
```

This is equivalent to adding *obs=value* as a keyword argument to *pyro.sample("z", ...)* in *model*.

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls)
- **data** – a dict or a *Trace*

Returns stochastic function decorated with a *ConditionMessenger*

do (*fn=None*, **args*, ***kwargs*)

Convenient wrapper of *DoMessenger*

Given a stochastic function with some sample statements and a dictionary of values at names, set the return values of those sites equal to the values as if they were hard-coded to those values and introduce fresh sample sites with the same names whose values do not propagate.

Composes freely with *condition()* to represent counterfactual distributions over potential outcomes. See Single World Intervention Graphs [1] for additional details and theory.

Consider the following Pyro program:

```
>>> def model(x):
...     s = pyro.param("s", torch.tensor(0.5))
...     z = pyro.sample("z", dist.Normal(x, s))
...     return z ** 2
```

To intervene with a value for site *z*, we can write

```
>>> intervened_model = pyro.poutine.do(model, data={"z": torch.tensor(1.)})
```

This is equivalent to replacing *z = pyro.sample("z", ...)* with *z = torch.tensor(1.)* and introducing a fresh sample site pyro.sample("z", ...) whose value is not used elsewhere.

References

[1] ***Single World Intervention Graphs: A Primer***, Thomas Richardson, James Robins

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls)
- **data** – a `dict` mapping sample site names to interventions

Returns stochastic function decorated with a *DoMessenger*

enum (*fn=None*, **args*, ***kwargs*)
Convenient wrapper of *EnumMessenger*

Enumerates in parallel over discrete sample sites marked `infer={"enumerate": "parallel"}`.

Parameters **first_available_dim** (*int*) – The first tensor dimension (counting from the right) that is available for parallel enumeration. This dimension and all dimensions left may be used internally by Pyro. This should be a negative integer or None.

escape (*fn=None*, **args*, ***kwargs*)
Convenient wrapper of *EscapeMessenger*

Messenger that does a nonlocal exit by raising a util.NonlocalExit exception

infer_config (*fn=None*, **args*, ***kwargs*)
Convenient wrapper of *InferConfigMessenger*

Given a callable *fn* that contains Pyro primitive calls and a callable *config_fn* taking a trace site and returning a dictionary, updates the value of the infer kwarg at a sample site to config_fn(site).

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls)
- **config_fn** – a callable taking a site and returning an infer dict

Returns stochastic function decorated with *InferConfigMessenger*

lift (*fn=None*, **args*, ***kwargs*)
Convenient wrapper of *LiftMessenger*

Given a stochastic function with param calls and a prior distribution, create a stochastic function where all param calls are replaced by sampling from prior. Prior should be a callable or a dict of names to callables.

Consider the following Pyro program:

```
>>> def model(x):
...     s = pyro.param("s", torch.tensor(0.5))
...     z = pyro.sample("z", dist.Normal(x, s))
...     return z ** 2
>>> lifted_model = pyro.poutine.lift(model, prior={"s": dist.Exponential(0.3)})
```

`lift` makes `param` statements behave like `sample` statements using the distributions in `prior`. In this example, site *s* will now behave as if it was replaced with `s = pyro.sample("s", dist.Exponential(0.3))`:

```
>>> tr = pyro.poutine.trace(lifted_model).get_trace(0.0)
>>> tr.nodes["s"]["type"] == "sample"
True
>>> tr2 = pyro.poutine.trace(lifted_model).get_trace(0.0)
>>> bool((tr2.nodes["s"]["value"] == tr.nodes["s"]["value"]).all())
False
```

Parameters

- **fn** – function whose parameters will be lifted to random values
- **prior** – prior function in the form of a Distribution or a dict of stochastic fns

Returns `fn` decorated with a *LiftMessenger*

markov (*fn=None*, *history=1*, *keep=False*, *dim=None*, *name=None*)
Markov dependency declaration.

This can be used in a variety of ways:

- as a context manager
- as a decorator for recursive functions
- as an iterator for markov chains

Parameters

- **history** (*int*) – The number of previous contexts visible from the current context. Defaults to 1. If zero, this is similar to `pyro.plate`.
- **keep** (*bool*) – If true, frames are replayable. This is important when branching: if `keep=True`, neighboring branches at the same level can depend on each other; if `keep=False`, neighboring branches are independent (conditioned on their share"
- **dim** (*int*) – An optional dimension to use for this independence index. Interface stub, behavior not yet implemented.
- **name** (*str*) – An optional unique name to help inference algorithms match `pyro.markov()` sites between models and guides. Interface stub, behavior not yet implemented.

mask (*fn=None*, **args*, ***kwargs*)
Convenient wrapper of *MaskMessenger*

Given a stochastic function with some batched sample statements and masking tensor, mask out some of the sample statements elementwise.

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls)
- **mask** (*torch.BoolTensor*) – a `{0,1}`-valued masking tensor (1 includes a site, 0 excludes a site)

Returns stochastic function decorated with a `MaskMessenger`

queue (*fn=None*, *queue=None*, *max_tries=None*, *extend_fn=None*, *escape_fn=None*, *num_samples=None*)
Used in sequential enumeration over discrete variables.

Given a stochastic function and a queue, return a return value from a complete trace in the queue.

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls)
- **queue** – a queue data structure like multiprocessing.Queue to hold partial traces
- **max_tries** – maximum number of attempts to compute a single complete trace
- **extend_fn** – function (possibly stochastic) that takes a partial trace and a site, and returns a list of extended traces
- **escape_fn** – function (possibly stochastic) that takes a partial trace and a site, and returns a boolean value to decide whether to exit
- **num_samples** – optional number of extended traces for extend_fn to return

Returns stochastic function decorated with poutine logic

reparam (*fn=None*, **args*, ***kwargs*)
Convenient wrapper of *ReparamMessenger*

Reparametrizes each affected sample site into one or more auxiliary sample sites followed by a deterministic transformation [1].

To specify reparameterizers, pass a `config` dict or callable to the constructor. See the *pyro.infer.reparam* module for available reparameterizers.

Note some reparameterizers can examine the `*args,**kwargs` inputs of functions they affect; these reparameterizers require using `poutine.reparam` as a decorator rather than as a context manager.

[1] Maria I. Gorinova, Dave Moore, Matthew D. Hoffman (2019) "Automatic Reparameterisation of Probabilistic Programs" https://arxiv.org/pdf/1906.03028.pdf

Parameters **config** (*dict or callable*) – Configuration, either a dict mapping site name to `Reparameterizer` , or a function mapping site to `Reparameterizer` or None.

replay (*fn=None*, **args*, ***kwargs*)
Convenient wrapper of *ReplayMessenger*

Given a callable that contains Pyro primitive calls, return a callable that runs the original, reusing the values at sites in trace at those sites in the new trace

Consider the following Pyro program:

```
>>> def model(x):
...     s = pyro.param("s", torch.tensor(0.5))
...     z = pyro.sample("z", dist.Normal(x, s))
...     return z ** 2
```

`replay` makes `sample` statements behave as if they had sampled the values at the corresponding sites in the trace:

```
>>> old_trace = pyro.poutine.trace(model).get_trace(1.0)
>>> replayed_model = pyro.poutine.replay(model, trace=old_trace)
>>> bool(replayed_model(0.0) == old_trace.nodes["_RETURN"]["value"])
True
```

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls)
- **trace** – a *Trace* data structure to replay against
- **params** – dict of names of param sites and constrained values in fn to replay against

Returns a stochastic function decorated with a *ReplayMessenger*

scale (*fn=None*, **args*, ***kwargs*)
Convenient wrapper of *ScaleMessenger*

Given a stochastic function with some sample statements and a positive scale factor, scale the score of all sample and observe sites in the function.

Consider the following Pyro program:

```
>>> def model(x):
...     s = pyro.param("s", torch.tensor(0.5))
...     z = pyro.sample("z", dist.Normal(x, s), obs=1.0)
...     return z ** 2
```

`scale` multiplicatively scales the log-probabilities of sample sites:

```
>>> scaled_model = pyro.poutine.scale(model, scale=0.5)
>>> scaled_tr = pyro.poutine.trace(scaled_model).get_trace(0.0)
>>> unscaled_tr = pyro.poutine.trace(model).get_trace(0.0)
>>> bool((scaled_tr.log_prob_sum() == 0.5 * unscaled_tr.log_prob_sum()).all())
True
```

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls)
- **scale** – a positive scaling factor

Returns stochastic function decorated with a *ScaleMessenger*

seed(*fn=None*, **args*, ***kwargs*)

Convenient wrapper of *SeedMessenger*

Handler to set the random number generator to a pre-defined state by setting its seed. This is the same as calling `pyro.set_rng_seed()` before the call to *fn*. This handler has no additional effect on primitive statements on the standard Pyro backend, but it might intercept `pyro.sample` calls in other backends. e.g. the NumPy backend.

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls).
- **rng_seed** (*int*) – rng seed.

trace(*fn=None*, **args*, ***kwargs*)

Convenient wrapper of *TraceMessenger*

Return a handler that records the inputs and outputs of primitive calls and their dependencies.

Consider the following Pyro program:

```
>>> def model(x):
...     s = pyro.param("s", torch.tensor(0.5))
...     z = pyro.sample("z", dist.Normal(x, s))
...     return z ** 2
```

We can record its execution using `trace` and use the resulting data structure to compute the log-joint probability of all of the sample sites in the execution or extract all parameters.

```
>>> trace = pyro.poutine.trace(model).get_trace(0.0)
>>> logp = trace.log_prob_sum()
>>> params = [trace.nodes[name]["value"].unconstrained() for name in trace.param_
↪nodes]
```

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls)
- **graph_type** – string that specifies the kind of graph to construct
- **param_only** – if true, only records params and not samples

Returns stochastic function decorated with a *TraceMessenger*

uncondition(*fn=None*, **args*, ***kwargs*)
Convenient wrapper of *UnconditionMessenger*

Messenger to force the value of observed nodes to be sampled from their distribution, ignoring observations.

config_enumerate(*guide=None*, *default='parallel'*, *expand=False*, *num_samples=None*, *tmc='diagonal'*)
Configures enumeration for all relevant sites in a guide. This is mainly used in conjunction with *TraceEnum_ELBO*.

When configuring for exhaustive enumeration of discrete variables, this configures all sample sites whose distribution satisfies `.has_enumerate_support == True`. When configuring for local parallel Monte Carlo sampling via `default="parallel", num_samples=n`, this configures all sample sites. This does not overwrite existing annotations `infer={"enumerate": ...}`.

This can be used as either a function:

```
guide = config_enumerate(guide)
```

or as a decorator:

```
@config_enumerate
def guide1(*args, **kwargs):
    ...

@config_enumerate(default="sequential", expand=True)
def guide2(*args, **kwargs):
    ...
```

Parameters

- **guide** (*callable*) – a pyro model that will be used as a guide in *SVI*.
- **default** (*str*) – Which enumerate strategy to use, one of "sequential", "parallel", or None. Defaults to "parallel".
- **expand** (*bool*) – Whether to expand enumerated sample values. See *enumerate_support()* for details. This only applies to exhaustive enumeration, where `num_samples=None`. If `num_samples` is not `None`, then this samples will always be expanded.
- **num_samples** (*int or None*) – if not `None`, use local Monte Carlo sampling rather than exhaustive enumeration. This makes sense for both continuous and discrete distributions.
- **tmc** (*string or None*) – "mixture" or "diagonal" strategies to use in Tensor Monte Carlo

Returns an annotated guide

Return type callable

8.2 Trace

class Trace(*graph_type='flat'*)
Bases: `object`

Graph data structure denoting the relationships amongst different pyro primitives in the execution trace.

An execution trace of a Pyro program is a record of every call to `pyro.sample()` and `pyro.param()` in a single execution of that program. Traces are directed graphs whose nodes represent primitive calls or input/output, and whose edges represent conditional dependence relationships between those primitive calls. They are created and populated by `poutine.trace`.

Each node (or site) in a trace contains the name, input and output value of the site, as well as additional metadata added by inference algorithms or user annotation. In the case of `pyro.sample`, the trace also includes the stochastic function at the site, and any observed data added by users.

Consider the following Pyro program:

```
>>> def model(x):
...     s = pyro.param("s", torch.tensor(0.5))
...     z = pyro.sample("z", dist.Normal(x, s))
...     return z ** 2
```

We can record its execution using `pyro.poutine.trace` and use the resulting data structure to compute the log-joint probability of all of the sample sites in the execution or extract all parameters.

```
>>> trace = pyro.poutine.trace(model).get_trace(0.0)
>>> logp = trace.log_prob_sum()
>>> params = [trace.nodes[name]["value"].unconstrained() for name in trace.param_
↪nodes]
```

We can also inspect or manipulate individual nodes in the trace. `trace.nodes` contains a `collections.OrderedDict` of site names and metadata corresponding to `x`, `s`, `z`, and the return value:

```
>>> list(name for name in trace.nodes.keys())  # doctest: +SKIP
["_INPUT", "s", "z", "_RETURN"]
```

Values of `trace.nodes` are dictionaries of node metadata:

```
>>> trace.nodes["z"]  # doctest: +SKIP
{'type': 'sample', 'name': 'z', 'is_observed': False,
 'fn': Normal(), 'value': tensor(0.6480), 'args': (), 'kwargs': {},
 'infer': {}, 'scale': 1.0, 'cond_indep_stack': (),
 'done': True, 'stop': False, 'continuation': None}
```

`'infer'` is a dictionary of user- or algorithm-specified metadata. `'args'` and `'kwargs'` are the arguments passed via `pyro.sample` to `fn.__call__` or `fn.log_prob`. `'scale'` is used to scale the log-probability of the site when computing the log-joint. `'cond_indep_stack'` contains data structures corresponding to `pyro.plate` contexts appearing in the execution. `'done'`, `'stop'`, and `'continuation'` are only used by Pyro's internals.

Parameters **graph_type** (*string*) – string specifying the kind of trace graph to construct

add_edge(*site1*, *site2*)

add_node(*site_name*, ***kwargs*)

Parameters **site_name** (*string*) – the name of the site to be added

Adds a site to the trace.

Raises an error when attempting to add a duplicate node instead of silently overwriting.

compute_log_prob(*site_filter=<function Trace.<lambda>>*)

Compute the site-wise log probabilities of the trace. Each `log_prob` has shape equal to the corresponding `batch_shape`. Each `log_prob_sum` is a scalar. Both computations are memoized.

compute_score_parts()
Compute the batched local score parts at each site of the trace. Each `log_prob` has shape equal to the corresponding `batch_shape`. Each `log_prob_sum` is a scalar. All computations are memoized.

copy()
Makes a shallow copy of self with nodes and edges preserved.

detach_()
Detach values (in-place) at each sample site of the trace.

edges

format_shapes(*title='Trace Shapes:'*, *last_site=None*)
Returns a string showing a table of the shapes of all sites in the trace.

iter_stochastic_nodes()

Returns an iterator over stochastic nodes in the trace.

log_prob_sum(*site_filter=<function Trace.<lambda>>*)
Compute the site-wise log probabilities of the trace. Each `log_prob` has shape equal to the corresponding `batch_shape`. Each `log_prob_sum` is a scalar. The computation of `log_prob_sum` is memoized.

Returns total log probability.

Return type torch.Tensor

nonreparam_stochastic_nodes

Returns a list of names of sample sites whose stochastic functions are not reparameterizable primitive distributions

observation_nodes

Returns a list of names of observe sites

pack_tensors(*plate_to_symbol=None*)
Computes packed representations of tensors in the trace. This should be called after *compute_log_prob()* or *compute_score_parts()*.

param_nodes

Returns a list of names of param sites

predecessors(*site_name*)

remove_node(*site_name*)

reparameterized_nodes

Returns a list of names of sample sites whose stochastic functions are reparameterizable primitive distributions

stochastic_nodes

Returns a list of names of sample sites

successors(*site_name*)

symbolize_dims(*plate_to_symbol=None*)
Assign unique symbols to all tensor dimensions.

topological_sort(*reverse=False*)
Return a list of nodes (site names) in topologically sorted order.

Parameters **reverse** (*bool*) – Return the list in reverse order.

Returns list of topologically sorted nodes (site names).

8.3 Runtime

exception NonlocalExit(*site*, **args*, ***kwargs*)
Bases: Exception

Exception for exiting nonlocally from poutine execution.

Used by poutine.EscapeMessenger to return site information.

reset_stack()
Reset the state of the frames remaining in the stack. Necessary for multiple re-executions in poutine.queue.

am_i_wrapped()
Checks whether the current computation is wrapped in a poutine. :returns: bool

apply_stack(*initial_msg*)
Execute the effect stack at a single site according to the following scheme:

1. For each Messenger in the stack from bottom to top, execute Messenger._process_message with the message; if the message field "stop" is True, stop; otherwise, continue
2. Apply default behavior (default_process_message) to finish remaining site execution
3. For each Messenger in the stack from top to bottom, execute _postprocess_message to update the message and internal messenger state with the site results
4. If the message field "continuation" is not None, call it with the message

Parameters **initial_msg** (*dict*) – the starting version of the trace site

Returns None

default_process_message(*msg*)
Default method for processing messages in inference.

Parameters **msg** – a message to be processed

Returns None

effectful(*fn=None*, *type=None*)

Parameters

- **fn** – function or callable that performs an effectful computation
- **type** (*str*) – the type label of the operation, e.g. *"sample"*

Wrapper for calling *apply_stack()* to apply any active effects.

8.4 Utilities

all_escape(*trace*, *msg*)

Parameters

- **trace** – a partial trace
- **msg** – the message at a Pyro primitive site

Returns boolean decision value

Utility function that checks if a site is not already in a trace.

Used by EscapeMessenger to decide whether to do a nonlocal exit at a site. Subroutine for approximately integrating out variables for variance reduction.

discrete_escape(*trace*, *msg*)

Parameters

- **trace** – a partial trace
- **msg** – the message at a Pyro primitive site

Returns boolean decision value

Utility function that checks if a sample site is discrete and not already in a trace.

Used by EscapeMessenger to decide whether to do a nonlocal exit at a site. Subroutine for integrating out discrete variables for variance reduction.

enable_validation(*is_validate*)

enum_extend(*trace*, *msg*, *num_samples=None*)

Parameters

- **trace** – a partial trace
- **msg** – the message at a Pyro primitive site
- **num_samples** – maximum number of extended traces to return.

Returns a list of traces, copies of input trace with one extra site

Utility function to copy and extend a trace with sites based on the input site whose values are enumerated from the support of the input site's distribution.

Used for exact inference and integrating out discrete variables.

is_validation_enabled()

mc_extend(*trace*, *msg*, *num_samples=None*)

Parameters

- **trace** – a partial trace
- **msg** – the message at a Pyro primitive site
- **num_samples** – maximum number of extended traces to return.

Returns a list of traces, copies of input trace with one extra site

Utility function to copy and extend a trace with sites based on the input site whose values are sampled from the input site's function.

Used for Monte Carlo marginalization of individual sample sites.

prune_subsample_sites(*trace*)
Copies and removes all subsample sites from a trace.

site_is_factor(*site*)
Determines whether a trace site originated from a factor statement.

site_is_subsample(*site*)
Determines whether a trace site originated from a subsample statement inside an *plate*.

8.5 Messengers

Messenger objects contain the implementations of the effects exposed by handlers. Advanced users may modify the implementations of messengers behind existing handlers or write new messengers that implement new effects and compose correctly with the rest of the library.

8.5.1 Messenger

class Messenger

Bases: object

Context manager class that modifies behavior and adds side effects to stochastic functions i.e. callables containing Pyro primitive statements.

This is the base Messenger class. It implements the default behavior for all Pyro primitives, so that the joint distribution induced by a stochastic function fn is identical to the joint distribution induced by `Messenger()(fn)`.

Class of transformers for messages passed during inference. Most inference operations are implemented in subclasses of this.

classmethod register(*fn=None*, *type=None*, *post=None*)

Parameters

- **fn** – function implementing operation
- **type** (*str*) – name of the operation (also passed to *effectful()*)
- **post** (*bool*) – if *True*, use this operation as postprocess

Dynamically add operations to an effect. Useful for generating wrappers for libraries.

Example:

```
@SomeMessengerClass.register
def some_function(msg)
    ...do_something...
    return msg
```

classmethod unregister(*fn=None*, *type=None*)

Parameters

- **fn** – function implementing operation
- **type** (*str*) – name of the operation (also passed to *effectful()*)

Dynamically remove operations from an effect. Useful for removing wrappers from libraries.

Example:

```
SomeMessengerClass.unregister(some_function, "name")
```

block_messengers(*predicate*)

EXPERIMENTAL Context manager to temporarily remove matching messengers from the _PYRO_STACK. Note this does not call the `.__exit__()` and `.__enter__()` methods.

This is useful to selectively block enclosing handlers.

Parameters **predicate** (*callable*) – A predicate mapping messenger instance to boolean. This mutes all messengers `m` for which `bool(predicate(m)) is True`.

Yields A list of matched messengers that are blocked.

8.5.2 BlockMessenger

class BlockMessenger(*hide_fn=None*, *expose_fn=None*, *hide_all=True*, *expose_all=False*, *hide=None*, *expose=None*, *hide_types=None*, *expose_types=None*)

Bases: *pyro.poutine.messenger.Messenger*

This handler selectively hides Pyro primitive sites from the outside world. Default behavior: block everything.

A site is hidden if at least one of the following holds:

0. `hide_fn(msg) is True` or `(not expose_fn(msg)) is True`
1. `msg["name"] in hide`
2. `msg["type"] in hide_types`
3. `msg["name"] not in expose and msg["type"] not in expose_types`
4. `hide`, `hide_types`, and `expose_types` are all `None`

For example, suppose the stochastic function fn has two sample sites "a" and "b". Then any effect outside of `BlockMessenger(fn, hide=["a"])` will not be applied to site "a" and will only see site "b":

```
>>> def fn():
...     a = pyro.sample("a", dist.Normal(0., 1.))
...     return pyro.sample("b", dist.Normal(a, 1.))
>>> fn_inner = pyro.poutine.trace(fn)
>>> fn_outer = pyro.poutine.trace(pyro.poutine.block(fn_inner, hide=["a"]))
>>> trace_inner = fn_inner.get_trace()
>>> trace_outer  = fn_outer.get_trace()
>>> "a" in trace_inner
True
>>> "a" in trace_outer
False
>>> "b" in trace_inner
True
>>> "b" in trace_outer
True
```

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls)
- **hide_fn** – function that takes a site and returns True to hide the site or False/None to expose it. If specified, all other parameters are ignored. Only specify one of hide_fn or expose_fn, not both.
- **expose_fn** – function that takes a site and returns True to expose the site or False/None to hide it. If specified, all other parameters are ignored. Only specify one of hide_fn or expose_fn, not both.
- **hide_all** (*bool*) – hide all sites
- **expose_all** (*bool*) – expose all sites normally
- **hide** (*list*) – list of site names to hide
- **expose** (*list*) – list of site names to be exposed while all others hidden
- **hide_types** (*list*) – list of site types to be hidden

- **expose_types** (*lits*) – list of site types to be exposed while all others hidden

Returns stochastic function decorated with a *BlockMessenger*

8.5.3 BroadcastMessenger

class BroadcastMessenger

Bases: *pyro.poutine.messenger.Messenger*

Automatically broadcasts the batch shape of the stochastic function at a sample site when inside a single or nested plate context. The existing *batch_shape* must be broadcastable with the size of the `plate` contexts installed in the *cond_indep_stack*.

Notice how *model_automatic_broadcast* below automates expanding of distribution batch shapes. This makes it easy to modularize a Pyro model as the sub-components are agnostic of the wrapping `plate` contexts.

```
>>> def model_broadcast_by_hand():
...     with IndepMessenger("batch", 100, dim=-2):
...         with IndepMessenger("components", 3, dim=-1):
...             sample = pyro.sample("sample", dist.Bernoulli(torch.ones(3) * 0.5)
...                                                 .expand_by(100))
...             assert sample.shape == torch.Size((100, 3))
...     return sample
```

```
>>> @poutine.broadcast
... def model_automatic_broadcast():
...     with IndepMessenger("batch", 100, dim=-2):
...         with IndepMessenger("components", 3, dim=-1):
...             sample = pyro.sample("sample", dist.Bernoulli(torch.tensor(0.5)))
...             assert sample.shape == torch.Size((100, 3))
...     return sample
```

8.5.4 CollapseMessenger

class CollapseMessenger(**args*, ***kwargs*)

Bases: *pyro.poutine.trace_messenger.TraceMessenger*

EXPERIMENTAL Collapses all sites in the context by lazily sampling and attempting to use conjugacy relations. If no conjugacy is known this will fail. Code using the results of sample sites must be written to accept Funsors rather than Tensors. This requires `funsor` to be installed.

Warning: This is not compatible with automatic guessing of `max_plate_nesting`. If any plates appear within the collapsed context, you should manually declare `max_plate_nesting` to your inference algorithm (e.g. `Trace_ELBO(max_plate_nesting=1)`).

8.5.5 ConditionMessenger

class ConditionMessenger(*data*)

Bases: *pyro.poutine.messenger.Messenger*

Given a stochastic function with some sample statements and a dictionary of observations at names, change the sample statements at those names into observes with those values.

Consider the following Pyro program:

```
>>> def model(x):
...     s = pyro.param("s", torch.tensor(0.5))
...     z = pyro.sample("z", dist.Normal(x, s))
...     return z ** 2
```

To observe a value for site *z*, we can write

```
>>> conditioned_model = pyro.poutine.condition(model, data={"z": torch.tensor(1.)}
↪)
```

This is equivalent to adding *obs=value* as a keyword argument to *pyro.sample("z", ...)* in *model*.

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls)
- **data** – a dict or a *Trace*

Returns stochastic function decorated with a *ConditionMessenger*

8.5.6 DoMessenger

class DoMessenger(*data*)

Bases: *pyro.poutine.messenger.Messenger*

Given a stochastic function with some sample statements and a dictionary of values at names, set the return values of those sites equal to the values as if they were hard-coded to those values and introduce fresh sample sites with the same names whose values do not propagate.

Composes freely with *condition()* to represent counterfactual distributions over potential outcomes. See Single World Intervention Graphs [1] for additional details and theory.

Consider the following Pyro program:

```
>>> def model(x):
...     s = pyro.param("s", torch.tensor(0.5))
...     z = pyro.sample("z", dist.Normal(x, s))
...     return z ** 2
```

To intervene with a value for site *z*, we can write

```
>>> intervened_model = pyro.poutine.do(model, data={"z": torch.tensor(1.)})
```

This is equivalent to replacing *z = pyro.sample("z", ...)* with *z = torch.tensor(1.)* and introducing a fresh sample site pyro.sample("z", ...) whose value is not used elsewhere.

References

[1] ***Single World Intervention Graphs: A Primer***, Thomas Richardson, James Robins

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls)
- **data** – a `dict` mapping sample site names to interventions

Returns stochastic function decorated with a *DoMessenger*

8.5.7 EnumMessenger

class EnumMessenger(*first_available_dim=None*)
Bases: *pyro.poutine.messenger.Messenger*

Enumerates in parallel over discrete sample sites marked `infer={"enumerate": "parallel"}`.

Parameters **first_available_dim** (*int*) – The first tensor dimension (counting from the right) that is available for parallel enumeration. This dimension and all dimensions left may be used internally by Pyro. This should be a negative integer or None.

enumerate_site(*msg*)

8.5.8 EscapeMessenger

class EscapeMessenger(*escape_fn*)
Bases: *pyro.poutine.messenger.Messenger*

Messenger that does a nonlocal exit by raising a util.NonlocalExit exception

8.5.9 IndepMessenger

class CondIndepStackFrame
Bases: *pyro.poutine.indep_messenger.CondIndepStackFrame*

vectorized

class IndepMessenger(*name=None*, *size=None*, *dim=None*, *device=None*)
Bases: *pyro.poutine.messenger.Messenger*

This messenger keeps track of stack of independence information declared by nested `plate` contexts. This information is stored in a `cond_indep_stack` at each sample/observe site for consumption by `TraceMessenger`.

Example:

```
x_axis = IndepMessenger('outer', 320, dim=-1)
y_axis = IndepMessenger('inner', 200, dim=-2)
with x_axis:
    x_noise = sample("x_noise", dist.Normal(loc, scale).expand_by([320]))
with y_axis:
    y_noise = sample("y_noise", dist.Normal(loc, scale).expand_by([200, 1]))
with x_axis, y_axis:
    xy_noise = sample("xy_noise", dist.Normal(loc, scale).expand_by([200, 320]))
```

indices

next_context()
Increments the counter.

8.5.10 InferConfigMessenger

class InferConfigMessenger(*config_fn*)
Bases: *pyro.poutine.messenger.Messenger*

Given a callable *fn* that contains Pyro primitive calls and a callable *config_fn* taking a trace site and returning a dictionary, updates the value of the infer kwarg at a sample site to config_fn(site).

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls)
- **config_fn** – a callable taking a site and returning an infer dict

Returns stochastic function decorated with *InferConfigMessenger*

8.5.11 LiftMessenger

class LiftMessenger(*prior*)

Bases: *pyro.poutine.messenger.Messenger*

Given a stochastic function with param calls and a prior distribution, create a stochastic function where all param calls are replaced by sampling from prior. Prior should be a callable or a dict of names to callables.

Consider the following Pyro program:

```
>>> def model(x):
...     s = pyro.param("s", torch.tensor(0.5))
...     z = pyro.sample("z", dist.Normal(x, s))
...     return z ** 2
>>> lifted_model = pyro.poutine.lift(model, prior={"s": dist.Exponential(0.3)})
```

`lift` makes `param` statements behave like `sample` statements using the distributions in `prior`. In this example, site *s* will now behave as if it was replaced with `s = pyro.sample("s", dist.Exponential(0.3))`:

```
>>> tr = pyro.poutine.trace(lifted_model).get_trace(0.0)
>>> tr.nodes["s"]["type"] == "sample"
True
>>> tr2 = pyro.poutine.trace(lifted_model).get_trace(0.0)
>>> bool((tr2.nodes["s"]["value"] == tr.nodes["s"]["value"]).all())
False
```

Parameters

- **fn** – function whose parameters will be lifted to random values
- **prior** – prior function in the form of a Distribution or a dict of stochastic fns

Returns `fn` decorated with a *LiftMessenger*

8.5.12 MarkovMessenger

class MarkovMessenger(*history=1*, *keep=False*, *dim=None*, *name=None*)

Bases: *pyro.poutine.reentrant_messenger.ReentrantMessenger*

Markov dependency declaration.

This is a statistical equivalent of a memory management arena.

Parameters

- **history** (*int*) – The number of previous contexts visible from the current context. Defaults to 1. If zero, this is similar to `pyro.plate`.
- **keep** (*bool*) – If true, frames are replayable. This is important when branching: if `keep=True`, neighboring branches at the same level can depend on each other; if

keep=False, neighboring branches are independent (conditioned on their shared ancestors).

- **dim** (*int*) – An optional dimension to use for this independence index. Interface stub, behavior not yet implemented.
- **name** (*str*) – An optional unique name to help inference algorithms match pyro.markov() sites between models and guides. Interface stub, behavior not yet implemented.

generator(*iterable*)

8.5.13 MaskMessenger

class MaskMessenger(*mask*)

Bases: *pyro.poutine.messenger.Messenger*

Given a stochastic function with some batched sample statements and masking tensor, mask out some of the sample statements elementwise.

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls)
- **mask** (*torch.BoolTensor*) – a {0,1}-valued masking tensor (1 includes a site, 0 excludes a site)

Returns stochastic function decorated with a MaskMessenger

8.5.14 PlateMessenger

class PlateMessenger(*name*, *size=None*, *subsample_size=None*, *subsample=None*, *dim=None*, *use_cuda=None*, *device=None*)

Bases: *pyro.poutine.subsample_messenger.SubsampleMessenger*

Swiss army knife of broadcasting amazingness: combines shape inference, independence annotation, and subsampling

block_plate(*name=None*, *dim=None*)

EXPERIMENTAL Context manager to temporarily block a single enclosing plate.

This is useful for sampling auxiliary variables or lazily sampling global variables that are needed in a plated context. For example the following models are equivalent:

Example:

```
def model_1(data):
    loc = pyro.sample("loc", dist.Normal(0, 1))
    with pyro.plate("data", len(data)):
        with block_plate("data"):
            scale = pyro.sample("scale", dist.LogNormal(0, 1))
        pyro.sample("x", dist.Normal(loc, scale))

def model_2(data):
    loc = pyro.sample("loc", dist.Normal(0, 1))
    scale = pyro.sample("scale", dist.LogNormal(0, 1))
    with pyro.plate("data", len(data)):
        pyro.sample("x", dist.Normal(loc, scale))
```

Parameters

- **name** (*str*) – Optional name of plate to match.
- **dim** (*int*) – Optional dim of plate to match. Must be negative.

Raises ValueError if no enclosing plate was found.

8.5.15 ReentrantMessenger

class ReentrantMessenger
Bases: *pyro.poutine.messenger.Messenger*

8.5.16 ReparamMessenger

class ReparamHandler(*msngr*, *fn*)
Bases: object

Reparameterization poutine.

class ReparamMessenger(*config*)
Bases: *pyro.poutine.messenger.Messenger*

Reparametrizes each affected sample site into one or more auxiliary sample sites followed by a deterministic transformation [1].

To specify reparameterizers, pass a `config` dict or callable to the constructor. See the *pyro.infer.reparam* module for available reparameterizers.

Note some reparameterizers can examine the `*args,**kwargs` inputs of functions they affect; these reparameterizers require using `poutine.reparam` as a decorator rather than as a context manager.

[1] Maria I. Gorinova, Dave Moore, Matthew D. Hoffman (2019) "Automatic Reparameterisation of Probabilistic Programs" https://arxiv.org/pdf/1906.03028.pdf

Parameters **config** (*dict or callable*) – Configuration, either a dict mapping site name to `Reparameterizer`, or a function mapping site to `Reparameterizer` or None.

8.5.17 ReplayMessenger

class ReplayMessenger(*trace=None*, *params=None*)
Bases: *pyro.poutine.messenger.Messenger*

Given a callable that contains Pyro primitive calls, return a callable that runs the original, reusing the values at sites in trace at those sites in the new trace

Consider the following Pyro program:

```
>>> def model(x):
...     s = pyro.param("s", torch.tensor(0.5))
...     z = pyro.sample("z", dist.Normal(x, s))
...     return z ** 2
```

`replay` makes `sample` statements behave as if they had sampled the values at the corresponding sites in the trace:

```
>>> old_trace = pyro.poutine.trace(model).get_trace(1.0)
>>> replayed_model = pyro.poutine.replay(model, trace=old_trace)
>>> bool(replayed_model(0.0) == old_trace.nodes["_RETURN"]["value"])
True
```

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls)
- **trace** – a *Trace* data structure to replay against
- **params** – dict of names of param sites and constrained values in fn to replay against

Returns a stochastic function decorated with a *ReplayMessenger*

8.5.18 ScaleMessenger

class ScaleMessenger(*scale*)

Bases: *pyro.poutine.messenger.Messenger*

Given a stochastic function with some sample statements and a positive scale factor, scale the score of all sample and observe sites in the function.

Consider the following Pyro program:

```
>>> def model(x):
...     s = pyro.param("s", torch.tensor(0.5))
...     z = pyro.sample("z", dist.Normal(x, s), obs=1.0)
...     return z ** 2
```

`scale` multiplicatively scales the log-probabilities of sample sites:

```
>>> scaled_model = pyro.poutine.scale(model, scale=0.5)
>>> scaled_tr = pyro.poutine.trace(scaled_model).get_trace(0.0)
>>> unscaled_tr = pyro.poutine.trace(model).get_trace(0.0)
>>> bool((scaled_tr.log_prob_sum() == 0.5 * unscaled_tr.log_prob_sum()).all())
True
```

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls)
- **scale** – a positive scaling factor

Returns stochastic function decorated with a *ScaleMessenger*

8.5.19 SeedMessenger

class SeedMessenger(*rng_seed*)

Bases: *pyro.poutine.messenger.Messenger*

Handler to set the random number generator to a pre-defined state by setting its seed. This is the same as calling `pyro.set_rng_seed()` before the call to *fn*. This handler has no additional effect on primitive statements on the standard Pyro backend, but it might intercept `pyro.sample` calls in other backends. e.g. the NumPy backend.

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls).
- **rng_seed** (*int*) – rng seed.

8.5.20 SubsampleMessenger

class SubsampleMessenger(*name*, *size=None*, *subsample_size=None*, *subsample=None*, *dim=None*, *use_cuda=None*, *device=None*)

Bases: *pyro.poutine.indep_messenger.IndepMessenger*

Extension of IndepMessenger that includes subsampling.

8.5.21 TraceMessenger

class TraceHandler(*msngr*, *fn*)

Bases: object

Execution trace poutine.

A TraceHandler records the input and output to every Pyro primitive and stores them as a site in a Trace(). This should, in theory, be sufficient information for every inference algorithm (along with the implicit computational graph in the Variables?)

We can also use this for visualization.

get_trace(**args*, ***kwargs*)

Returns data structure

Return type *pyro.poutine.Trace*

Helper method for a very common use case. Calls this poutine and returns its trace instead of the function's return value.

trace

class TraceMessenger(*graph_type=None*, *param_only=None*)

Bases: *pyro.poutine.messenger.Messenger*

Return a handler that records the inputs and outputs of primitive calls and their dependencies.

Consider the following Pyro program:

```
>>> def model(x):
...     s = pyro.param("s", torch.tensor(0.5))
...     z = pyro.sample("z", dist.Normal(x, s))
...     return z ** 2
```

We can record its execution using `trace` and use the resulting data structure to compute the log-joint probability of all of the sample sites in the execution or extract all parameters.

```
>>> trace = pyro.poutine.trace(model).get_trace(0.0)
>>> logp = trace.log_prob_sum()
>>> params = [trace.nodes[name]["value"].unconstrained() for name in trace.param_
↪nodes]
```

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls)
- **graph_type** – string that specifies the kind of graph to construct

- **param_only** – if true, only records params and not samples

Returns stochastic function decorated with a *TraceMessenger*

get_trace()

Returns data structure

Return type *pyro.poutine.Trace*

Helper method for a very common use case. Returns a shallow copy of `self.trace`.

identify_dense_edges(*trace*)

Modifies a trace in-place by adding all edges based on the *cond_indep_stack* information stored at each site.

8.5.22 UnconditionMessenger

class UnconditionMessenger

Bases: *pyro.poutine.messenger.Messenger*

Messenger to force the value of observed nodes to be sampled from their distribution, ignoring observations.

CHAPTER 9

Miscellaneous Ops

The `pyro.ops` module implements tensor utilities that are mostly independent of the rest of Pyro.

9.1 Utilities for HMC

class DualAveraging(*prox_center=0*, *t0=10*, *kappa=0.75*, *gamma=0.05*)

Bases: `object`

Dual Averaging is a scheme to solve convex optimization problems. It belongs to a class of subgradient methods which uses subgradients to update parameters (in primal space) of a model. Under some conditions, the averages of generated parameters during the scheme are guaranteed to converge to an optimal value. However, a counter-intuitive aspect of traditional subgradient methods is "new subgradients enter the model with decreasing weights" (see [1]). Dual Averaging scheme solves that phenomenon by updating parameters using weights equally for subgradients (which lie in a dual space), hence we have the name "dual averaging".

This class implements a dual averaging scheme which is adapted for Markov chain Monte Carlo (MCMC) algorithms. To be more precise, we will replace subgradients by some statistics calculated during an MCMC trajectory. In addition, introducing some free parameters such as `t0` and `kappa` is helpful and still guarantees the convergence of the scheme.

References

[1] *Primal-dual subgradient methods for convex problems*, Yurii Nesterov

[2] *The No-U-turn sampler: adaptively setting path lengths in Hamiltonian Monte Carlo*, Matthew D. Hoffman, Andrew Gelman

Parameters

- **prox_center** (*float*) – A "prox-center" parameter introduced in [1] which pulls the primal sequence towards it.
- **t0** (*float*) – A free parameter introduced in [2] that stabilizes the initial steps of the scheme.

- **kappa** (*float*) – A free parameter introduced in [2] that controls the weights of steps of the scheme. For a small `kappa`, the scheme will quickly forget states from early steps. This should be a number in $(0.5, 1]$.
- **gamma** (*float*) – A free parameter which controls the speed of the convergence of the scheme.

reset()

step(*g*)

Updates states of the scheme given a new statistic/subgradient `g`.

Parameters **g** (*float*) – A statistic calculated during an MCMC trajectory or subgradient.

get_state()

Returns the latest x_t and average of $\{x_i\}_{i=1}^{t}$ in primal space.

velocity_verlet(*z*, *r*, *potential_fn*, *kinetic_grad*, *step_size*, *num_steps=1*, *z_grads=None*)

Second order symplectic integrator that uses the velocity verlet algorithm.

Parameters

- **z** (*dict*) – dictionary of sample site names and their current values (type `Tensor`).
- **r** (*dict*) – dictionary of sample site names and corresponding momenta (type `Tensor`).
- **potential_fn** (*callable*) – function that returns potential energy given `z` for each sample site. The negative gradient of the function with respect to `z` determines the rate of change of the corresponding sites' momenta `r`.
- **kinetic_grad** (*callable*) – a function calculating gradient of kinetic energy w.r.t. momentum variable.
- **step_size** (*float*) – step size for each time step iteration.
- **num_steps** (*int*) – number of discrete time steps over which to integrate.
- **z_grads** (*torch.Tensor*) – optional gradients of potential energy at current `z`.

Return tuple (z_next, r_next, z_grads, potential_energy) next position and momenta, together with the potential energy and its gradient w.r.t. `z_next`.

potential_grad(*potential_fn*, *z*)

Gradient of *potential_fn* w.r.t. parameters z.

Parameters

- **potential_fn** – python callable that takes in a dictionary of parameters and returns the potential energy.
- **z** (*dict*) – dictionary of parameter values keyed by site name.

Returns tuple of *(z_grads, potential_energy)*, where *z_grads* is a dictionary with the same keys as *z* containing gradients and potential_energy is a torch scalar.

class WelfordCovariance(*diagonal=True*)

Bases: `object`

Implements Welford's online scheme for estimating (co)variance (see [1]). Useful for adapting diagonal and dense mass structures for HMC.

References

[1] *The Art of Computer Programming*, Donald E. Knuth

reset()

update(*sample*)

get_covariance(*regularize=True*)

class WelfordArrowheadCovariance(*head_size=0*)
Bases: object

Likes *WelfordCovariance* but generalized to the arrowhead structure.

reset()

update(*sample*)

get_covariance(*regularize=True*)
Gets the covariance in arrowhead form: (top, bottom_diag) where *top = cov[:head_size]* and *bottom_diag = cov.diag()[head_size:]*.

9.2 Newton Optimizers

newton_step(*loss*, *x*, *trust_radius=None*)
Performs a Newton update step to minimize loss on a batch of variables, optionally constraining to a trust region [1].

This is especially usful because the final solution of newton iteration is differentiable wrt the inputs, even when all but the final `x` is detached, due to this method's quadratic convergence [2]. `loss` must be twice-differentiable as a function of `x`. If `loss` is `2+d`-times differentiable, then the return value of this function is `d`-times differentiable.

When `loss` is interpreted as a negative log probability density, then the return values `mode,cov` of this function can be used to construct a Laplace approximation `MultivariateNormal(mode,cov)`.

Warning: Take care to detach the result of this function when used in an optimization loop. If you forget to detach the result of this function during optimization, then backprop will propagate through the entire iteration process, and worse will compute two extra derivatives for each step.

Example use inside a loop:

```
x = torch.zeros(1000, 2)  # arbitrary initial value
for step in range(100):
    x = x.detach()           # block gradients through previous steps
    x.requires_grad = True   # ensure loss is differentiable wrt x
    loss = my_loss_function(x)
    x = newton_step(loss, x, trust_radius=1.0)
# the final x is still differentiable
```

[1] Yuan, Ya-xiang. Iciam. Vol. 99. 2000. "A review of trust region algorithms for optimization." ftp://ftp.cc.ac.cn/pub/yyx/papers/p995.pdf

[2] Christianson, Bruce. Optimization Methods and Software 3.4 (1994) "Reverse accumulation and attractive fixed points." http://uhra.herts.ac.uk/bitstream/handle/2299/4338/903839.pdf

Parameters

- **loss** (*torch.Tensor*) – A scalar function of `x` to be minimized.
- **x** (*torch.Tensor*) – A dependent variable of shape `(N, D)` where `N` is the batch size and `D` is a small number.

- **trust_radius** (*float*) – An optional trust region trust_radius. The updated value `mode` of this function will be within `trust_radius` of the input `x`.

Returns A pair `(mode, cov)` where `mode` is an updated tensor of the same shape as the original value `x`, and `cov` is an esitmate of the covariance DxD matrix with `cov.shape == x.shape[:-1] + (D,D)`.

Return type tuple

newton_step_1d(*loss*, *x*, *trust_radius=None*)

Performs a Newton update step to minimize loss on a batch of 1-dimensional variables, optionally regularizing to constrain to a trust region.

See *newton_step()* for details.

Parameters

- **loss** (*torch.Tensor*) – A scalar function of `x` to be minimized.
- **x** (*torch.Tensor*) – A dependent variable with rightmost size of 1.
- **trust_radius** (*float*) – An optional trust region trust_radius. The updated value `mode` of this function will be within `trust_radius` of the input `x`.

Returns A pair `(mode, cov)` where `mode` is an updated tensor of the same shape as the original value `x`, and `cov` is an esitmate of the covariance 1x1 matrix with `cov.shape == x.shape[:-1] + (1,1)`.

Return type tuple

newton_step_2d(*loss*, *x*, *trust_radius=None*)

Performs a Newton update step to minimize loss on a batch of 2-dimensional variables, optionally regularizing to constrain to a trust region.

See *newton_step()* for details.

Parameters

- **loss** (*torch.Tensor*) – A scalar function of `x` to be minimized.
- **x** (*torch.Tensor*) – A dependent variable with rightmost size of 2.
- **trust_radius** (*float*) – An optional trust region trust_radius. The updated value `mode` of this function will be within `trust_radius` of the input `x`.

Returns A pair `(mode, cov)` where `mode` is an updated tensor of the same shape as the original value `x`, and `cov` is an esitmate of the covariance 2x2 matrix with `cov.shape == x.shape[:-1] + (2,2)`.

Return type tuple

newton_step_3d(*loss*, *x*, *trust_radius=None*)

Performs a Newton update step to minimize loss on a batch of 3-dimensional variables, optionally regularizing to constrain to a trust region.

See *newton_step()* for details.

Parameters

- **loss** (*torch.Tensor*) – A scalar function of `x` to be minimized.
- **x** (*torch.Tensor*) – A dependent variable with rightmost size of 2.
- **trust_radius** (*float*) – An optional trust region trust_radius. The updated value `mode` of this function will be within `trust_radius` of the input `x`.

Returns A pair `(mode, cov)` where `mode` is an updated tensor of the same shape as the original value `x`, and `cov` is an esitmate of the covariance 3x3 matrix with `cov.shape == x.shape[:-1] + (3,3)`.

Return type tuple

9.3 Special Functions

safe_log(*x*)

Like `torch.log()` but avoids infinite gradients at log(0) by clamping them to at most `1 / finfo.eps`.

log_beta(*x*, *y*, *tol=0.0*)

Computes log Beta function.

When `tol >= 0.02` this uses a shifted Stirling's approximation to the log Beta function. The approximation adapts Stirling's approximation of the log Gamma function:

```
lgamma(z)  (z - 1/2) * log(z) - z + log(2 * pi) / 2
```

to approximate the log Beta function:

```
log_beta(x, y)  ((x-1/2) * log(x) + (y-1/2) * log(y)
                   - (x+y-1/2) * log(x+y) + log(2*pi)/2)
```

The approximation additionally improves accuracy near zero by iteratively shifting the log Gamma approximation using the recursion:

```
lgamma(x) = lgamma(x + 1) - log(x)
```

If this recursion is applied `n` times, then absolute error is bounded by `error < 0.082 / n < tol`, thus we choose `n` based on the user provided `tol`.

Parameters

- **x** (*torch.Tensor*) – A positive tensor.
- **y** (*torch.Tensor*) – A positive tensor.
- **tol** (*float*) – Bound on maximum absolute error. Defaults to 0.1. For very small `tol`, this function simply defers to *log_beta()*.

Return type torch.Tensor

log_binomial(*n*, *k*, *tol=0.0*)

Computes log binomial coefficient.

When `tol >= 0.02` this uses a shifted Stirling's approximation to the log Beta function via *log_beta()*.

Parameters

- **n** (*torch.Tensor*) – A nonnegative integer tensor.
- **k** (*torch.Tensor*) – An integer tensor ranging in `[0, n]`.

Return type torch.Tensor

9.4 Tensor Utilities

block_diag_embed(*mat*)
Takes a tensor of shape (..., B, M, N) and returns a block diagonal tensor of shape (..., B x M, B x N).

Parameters **mat** (*torch.Tensor*) – an input tensor with 3 or more dimensions

Returns torch.Tensor a block diagonal tensor with dimension *m.dim() - 1*

block_diagonal(*mat*, *block_size*)
Takes a block diagonal tensor of shape (..., B x M, B x N) and returns a tensor of shape (..., B, M, N).

Parameters

- **mat** (*torch.Tensor*) – an input tensor with 2 or more dimensions
- **block_size** (*int*) – the number of blocks B.

Returns torch.Tensor a tensor with dimension *mat.dim() + 1*

periodic_repeat(*tensor*, *size*, *dim*)
Repeat a `period`-sized tensor up to given `size`. For example:

```
>>> x = torch.tensor([[1, 2, 3], [4, 5, 6]])
>>> periodic_repeat(x, 4, 0)
tensor([[1, 2, 3],
        [4, 5, 6],
        [1, 2, 3],
        [4, 5, 6]])
>>> periodic_repeat(x, 4, 1)
tensor([[1, 2, 3, 1],
        [4, 5, 6, 4]])
```

This is useful for computing static seasonality in time series models.

Parameters

- **tensor** (*torch.Tensor*) – A tensor of differences.
- **size** (*int*) – Desired size of the result along dimension `dim`.
- **dim** (*int*) – The tensor dimension along which to repeat.

periodic_cumsum(*tensor*, *period*, *dim*)
Compute periodic cumsum along a given dimension. For example if dim=0:

```
for t in range(period):
    assert result[t] == tensor[t]
for t in range(period, len(tensor)):
    assert result[t] == tensor[t] + result[t - period]
```

This is useful for computing drifting seasonality in time series models.

Parameters

- **tensor** (*torch.Tensor*) – A tensor of differences.
- **period** (*int*) – The period of repetition.
- **dim** (*int*) – The tensor dimension along which to accumulate.

periodic_features(*duration*, *max_period=None*, *min_period=None*, ***options*)
Create periodic (sin,cos) features from `max_period` down to `min_period`.

This is useful in time series models where long uneven seasonality can be treated via regression. When only `max_period` is specified this generates periodic features at all length scales. When also `min_period` is specified this generates periodic features at large length scales, but omits high frequency features. This is useful when combining regression for long seasonality with other techniques like *periodic_repeat()* and *periodic_cumsum()* for short time scales. For example, to combine regress yearly seasonality down to the scale of one week one could set `max_period=365.25` and `min_period=7`.

Parameters

- **duration** (*int*) – Number of discrete time steps.
- **max_period** (*float*) – Optional max period, defaults to `duration`.
- **min_period** (*float*) – Optional min period (exclusive), defaults to 2 = Nyquist cutoff.
- ****options** – Tensor construction options, e.g. `dtype` and `device`.

Returns A `(duration, 2 * ceil(max_period / min_period) - 2)`-shaped tensor of features normalized to lie in [-1,1].

Return type Tensor

next_fast_len(*size*)

Returns the next largest number `n >= size` whose prime factors are all 2, 3, or 5. These sizes are efficient for fast fourier transforms. Equivalent to `scipy.fftpack.next_fast_len()`.

Parameters **size** (*int*) – A positive number.

Returns A possibly larger number.

Rtype int

convolve(*signal*, *kernel*, *mode='full'*)

Computes the 1-d convolution of signal by kernel using FFTs. The two arguments should have the same rightmost dim, but may otherwise be arbitrarily broadcastable.

Parameters

- **signal** (*torch.Tensor*) – A signal to convolve.
- **kernel** (*torch.Tensor*) – A convolution kernel.
- **mode** (*str*) – One of: 'full', 'valid', 'same'.

Returns A tensor with broadcasted shape. Letting `m = signal.size(-1)` and `n = kernel.size(-1)`, the rightmost size of the result will be: `m + n - 1` if mode is 'full'; `max(m, n) - min(m, n) + 1` if mode is 'valid'; or `max(m, n)` if mode is 'same'.

Rtype torch.Tensor

repeated_matmul(*M*, *n*)

Takes a batch of matrices *M* as input and returns the stacked result of doing the *n*-many matrix multiplications $M, M^2, \ldots, M^n$. Parallel cost is logarithmic in *n*.

Parameters

- **M** (*torch.Tensor*) – A batch of square tensors of shape (..., N, N).
- **n** (*int*) – The order of the largest product M^n

Returns torch.Tensor A batch of square tensors of shape (n, ..., N, N)

dct(*x*, *dim=-1*)

Discrete cosine transform of type II, scaled to be orthonormal.

This is the inverse of `idct_ii()`, and is equivalent to `scipy.fftpack.dct()` with `norm="ortho"`.

Parameters

- **x** (*Tensor*) – The input signal.
- **dim** (*int*) – Dimension along which to compute DCT.

Return type Tensor

idct(*x*, *dim=-1*)

Inverse discrete cosine transform of type II, scaled to be orthonormal.

This is the inverse of `dct_ii()`, and is equivalent to `scipy.fftpack.idct()` with `norm="ortho"`.

Parameters

- **x** (*Tensor*) – The input signal.
- **dim** (*int*) – Dimension along which to compute DCT.

Return type Tensor

haar_transform(*x*)

Discrete Haar transform.

Performs a Haar transform along the final dimension. This is the inverse of *inverse_haar_transform()*.

Parameters **x** (*Tensor*) – The input signal.

Return type Tensor

inverse_haar_transform(*x*)

Performs an inverse Haar transform along the final dimension. This is the inverse of *haar_transform()*.

Parameters **x** (*Tensor*) – The input signal.

Return type Tensor

cholesky(*x*)

cholesky_solve(*x*, *y*)

matmul(*x*, *y*)

matvecmul(*x*, *y*)

triangular_solve(*x*, *y*, *upper=False*, *transpose=False*)

precision_to_scale_tril(*P*)

9.5 Tensor Indexing

index(*tensor*, *args*)

Indexing with nested tuples.

See also the convenience wrapper *Index*.

This is useful for writing indexing code that is compatible with multiple interpretations, e.g. scalar evaluation, vectorized evaluation, or reshaping.

For example suppose `x` is a parameter with `x.dim() == 2` and we wish to generalize the expression `x[..., t]` where `t` can be any of:

- a scalar `t=1` as in `x[..., 1]`;
- a slice `t=slice(None)` equivalent to `x[..., :]`; or

- a reshaping operation `t=(Ellipsis, None)` equivalent to `x.unsqueeze(-1)`.

While naive indexing would work for the first two , the third example would result in a nested tuple `(Ellipsis, (Ellipsis, None))`. This helper flattens that nested tuple and combines consecutive `Ellipsis`.

Parameters

- **tensor** (*torch.Tensor*) – A tensor to be indexed.
- **args** (*tuple*) – An index, as args to `__getitem__`.

Returns A flattened interpetation of `tensor[args]`.

Return type torch.Tensor

class Index(*tensor*)

Bases: `object`

Convenience wrapper around *index()*.

The following are equivalent:

```
Index(x)[..., i, j, :]
index(x, (Ellipsis, i, j, slice(None)))
```

Parameters **tensor** (*torch.Tensor*) – A tensor to be indexed.

Returns An object with a special `__getitem__()` method.

vindex(*tensor*, *args*)

Vectorized advanced indexing with broadcasting semantics.

See also the convenience wrapper *Vindex*.

This is useful for writing indexing code that is compatible with batching and enumeration, especially for selecting mixture components with discrete random variables.

For example suppose `x` is a parameter with `x.dim() == 3` and we wish to generalize the expression `x[i, :, j]` from integer `i,j` to tensors `i,j` with batch dims and enum dims (but no event dims). Then we can write the generalize version using *Vindex*

```
xij = Vindex(x)[i, :, j]

batch_shape = broadcast_shape(i.shape, j.shape)
event_shape = (x.size(1),)
assert xij.shape == batch_shape + event_shape
```

To handle the case when `x` may also contain batch dimensions (e.g. if `x` was sampled in a plated context as when using vectorized particles), *vindex()* uses the special convention that `Ellipsis` denotes batch dimensions (hence `...` can appear only on the left, never in the middle or in the right). Suppose `x` has event dim 3. Then we can write:

```
old_batch_shape = x.shape[:-3]
old_event_shape = x.shape[-3:]

xij = Vindex(x)[..., i, :, j]   # The ... denotes unknown batch shape.

new_batch_shape = broadcast_shape(old_batch_shape, i.shape, j.shape)
new_event_shape = (x.size(1),)
assert xij.shape = new_batch_shape + new_event_shape
```

Note that this special handling of `Ellipsis` differs from the NEP [1].

Formally, this function assumes:

1. Each arg is either `Ellipsis`, `slice(None)`, an integer, or a batched `torch.LongTensor` (i.e. with empty event shape). This function does not support Nontrivial slices or `torch.BoolTensor` masks. `Ellipsis` can only appear on the left as `args[0]`.
2. If `args[0] is not Ellipsis` then `tensor` is not batched, and its event dim is equal to `len(args)`.
3. If `args[0] is Ellipsis` then `tensor` is batched and its event dim is equal to `len(args[1:])`. Dims of `tensor` to the left of the event dims are considered batch dims and will be broadcasted with dims of tensor args.

Note that if none of the args is a tensor with `.dim() > 0`, then this function behaves like standard indexing:

```
if not any(isinstance(a, torch.Tensor) and a.dim() for a in args):
    assert Vindex(x)[args] == x[args]
```

References

[1] https://www.numpy.org/neps/nep-0021-advanced-indexing.html introduces `vindex` as a helper for vectorized indexing. The Pyro implementation is similar to the proposed notation `x.vindex[]` except for slightly different handling of `Ellipsis`.

Parameters

- **tensor** (*torch.Tensor*) – A tensor to be indexed.
- **args** (*tuple*) – An index, as args to `__getitem__`.

Returns A nonstandard interpetation of `tensor[args]`.

Return type torch.Tensor

class Vindex(*tensor*)

Bases: `object`

Convenience wrapper around *vindex()*.

The following are equivalent:

```
Vindex(x)[..., i, j, :]
vindex(x, (Ellipsis, i, j, slice(None)))
```

Parameters **tensor** (*torch.Tensor*) – A tensor to be indexed.

Returns An object with a special `__getitem__()` method.

9.6 Tensor Contraction

contract_expression(*equation*, **shapes*, ***kwargs*)

Wrapper around `opt_einsum.contract_expression()` that optionally uses Pyro's cheap optimizer and optionally caches contraction paths.

Parameters **cache_path** (*bool*) – whether to cache the contraction path. Defaults to True.

contract(*equation*, **operands*, ***kwargs*)
Wrapper around `opt_einsum.contract()` that optionally uses Pyro's cheap optimizer and optionally caches contraction paths.

Parameters **cache_path** (*bool*) – whether to cache the contraction path. Defaults to True.

einsum(*equation*, **operands*, ***kwargs*)
Generalized plated sum-product algorithm via tensor variable elimination.

This generalizes *contract()* in two ways:

1. Multiple outputs are allowed, and intermediate results can be shared.
2. Inputs and outputs can be plated along symbols given in `plates`; reductions along `plates` are product reductions.

The best way to understand this function is to try the examples below, which show how *einsum()* calls can be implemented as multiple calls to *contract()* (which is generally more expensive).

To illustrate multiple outputs, note that the following are equivalent:

```
z1, z2, z3 = einsum('ab,bc->a,b,c', x, y)  # multiple outputs

z1 = contract('ab,bc->a', x, y)
z2 = contract('ab,bc->b', x, y)
z3 = contract('ab,bc->c', x, y)
```

To illustrate plated inputs, note that the following are equivalent:

```
assert len(x) == 3 and len(y) == 3
z = einsum('ab,ai,bi->b', w, x, y, plates='i')

z = contract('ab,a,a,a,b,b,b->b', w, *x, *y)
```

When a sum dimension *a* always appears with a plate dimension *i*, then *a* corresponds to a distinct symbol for each slice of *a*. Thus the following are equivalent:

```
assert len(x) == 3 and len(y) == 3
z = einsum('ai,ai->', x, y, plates='i')

z = contract('a,b,c,a,b,c->', *x, *y)
```

When such a sum dimension appears in the output, it must be accompanied by all of its plate dimensions, e.g. the following are equivalent:

```
assert len(x) == 3 and len(y) == 3
z = einsum('abi,abi->bi', x, y, plates='i')

z0 = contract('ab,ac,ad,ab,ac,ad->b', *x, *y)
z1 = contract('ab,ac,ad,ab,ac,ad->c', *x, *y)
z2 = contract('ab,ac,ad,ab,ac,ad->d', *x, *y)
z = torch.stack([z0, z1, z2])
```

Note that each plate slice through the output is multilinear in all plate slices through all inptus, thus e.g. batch matrix multiply would be implemented *without* `plates`, so the following are all equivalent:

```
xy = einsum('abc,acd->abd', x, y, plates='')
xy = torch.stack([xa.mm(ya) for xa, ya in zip(x, y)])
xy = torch.bmm(x, y)
```

Among all valid equations, some computations are polynomial in the sizes of the input tensors and other computations are exponential in the sizes of the input tensors. This function raises `NotImplementedError` whenever the computation is exponential.

Parameters

- **equation** (*str*) – An einsum equation, optionally with multiple outputs.
- **operands** (*torch.Tensor*) – A collection of tensors.
- **plates** (*str*) – An optional string of plate symbols.
- **backend** (*str*) – An optional einsum backend, defaults to 'torch'.
- **cache** (*dict*) – An optional `shared_intermediates()` cache.
- **modulo_total** (*bool*) – Optionally allow einsum to arbitrarily scale each result plate, which can significantly reduce computation. This is safe to set whenever each result plate denotes a nonnormalized probability distribution whose total is not of interest.

Returns a tuple of tensors of requested shape, one entry per output.

Return type tuple

Raises

- **ValueError** – if tensor sizes mismatch or an output requests a plated dim without that dim's plates.
- **NotImplementedError** – if contraction would have cost exponential in the size of any input tensor.

ubersum(*equation*, **operands*, ***kwargs*)
Deprecated, use *einsum()* instead.

9.7 Gaussian Contraction

class Gaussian(*log_normalizer*, *info_vec*, *precision*)
Bases: `object`

Non-normalized Gaussian distribution.

This represents an arbitrary semidefinite quadratic function, which can be interpreted as a rank-deficient scaled Gaussian distribution. The precision matrix may have zero eigenvalues, thus it may be impossible to work directly with the covariance matrix.

Parameters

- **log_normalizer** (*torch.Tensor*) – a normalization constant, which is mainly used to keep track of normalization terms during contractions.
- **info_vec** (*torch.Tensor*) – information vector, which is a scaled version of the mean `info_vec = precision @ mean`. We use this represention to make gaussian contraction fast and stable.
- **precision** (*torch.Tensor*) – precision matrix of this gaussian.

dim()

batch_shape

expand(*batch_shape*)

reshape(*batch_shape*)

__getitem__(*index*)
Index into the batch_shape of a Gaussian.

static cat(*parts*, *dim=0*)
Concatenate a list of Gaussians along a given batch dimension.

event_pad(*left=0*, *right=0*)
Pad along event dimension.

event_permute(*perm*)
Permute along event dimension.

__add__(*other*)
Adds two Gaussians in log-density space.

log_density(*value*)
Evaluate the log density of this Gaussian at a point value:

```
-0.5 * value.T @ precision @ value + value.T @ info_vec + log_normalizer
```

This is mainly used for testing.

rsample(*sample_shape=torch.Size([])*)
Reparameterized sampler.

condition(*value*)
Condition this Gaussian on a trailing subset of its state. This should satisfy:

```
g.condition(y).dim() == g.dim() - y.size(-1)
```

Note that since this is a non-normalized Gaussian, we include the density of `y` in the result. Thus *condition()* is similar to a `functools.partial` binding of arguments:

```
left = x[..., :n]
right = x[..., n:]
g.log_density(x) == g.condition(right).log_density(left)
```

left_condition(*value*)
Condition this Gaussian on a leading subset of its state. This should satisfy:

```
g.condition(y).dim() == g.dim() - y.size(-1)
```

Note that since this is a non-normalized Gaussian, we include the density of `y` in the result. Thus *condition()* is similar to a `functools.partial` binding of arguments:

```
left = x[..., :n]
right = x[..., n:]
g.log_density(x) == g.left_condition(left).log_density(right)
```

marginalize(*left=0*, *right=0*)
Marginalizing out variables on either side of the event dimension:

```
g.marginalize(left=n).event_logsumexp() = g.logsumexp()
g.marginalize(right=n).event_logsumexp() = g.logsumexp()
```

and for data `x`:

g.condition(x).event_logsumexp() = g.marginalize(left=g.dim() - x.size(-1)).log_density(x)

event_logsumexp()
Integrates out all latent state (i.e. operating on event dimensions).

class AffineNormal(*matrix*, *loc*, *scale*)
Bases: object

Represents a conditional diagonal normal distribution over a random variable Y whose mean is an affine function of a random variable X. The likelihood of X is thus:

```
AffineNormal(matrix, loc, scale).condition(y).log_density(x)
```

which is equivalent to:

```
Normal(x @ matrix + loc, scale).to_event(1).log_prob(y)
```

Parameters

- **matrix** (*torch.Tensor*) – A transformation from X to Y. Should have rightmost shape (x_dim, y_dim).
- **loc** (*torch.Tensor*) – A constant offset for Y's mean. Should have rightmost shape (y_dim,).
- **scale** (*torch.Tensor*) – Standard deviation for Y. Should have rightmost shape (y_dim,).

batch_shape

condition(*value*)

left_condition(*value*)
If value.size(-1) == x_dim, this returns a Normal distribution with event_dim=1. After applying this method, the cost to draw a sample is O(y_dim) instead of O(y_dim ** 3).

rsample(*sample_shape=torch.Size([])*)
Reparameterized sampler.

to_gaussian()

expand(*batch_shape*)

reshape(*batch_shape*)

__getitem__(*index*)

event_permute(*perm*)

__add__(*other*)

marginalize(*left=0*, *right=0*)

mvn_to_gaussian(*mvn*)
Convert a MultivariateNormal distribution to a Gaussian.

Parameters **mvn** (*MultivariateNormal*) – A multivariate normal distribution.

Returns An equivalent Gaussian object.

Return type *Gaussian*

matrix_and_mvn_to_gaussian(*matrix*, *mvn*)
Convert a noisy affine function to a Gaussian. The noisy affine function is defined as:

```
y = x @ matrix + mvn.sample()
```

Parameters

- **matrix** (*Tensor*) – A matrix with rightmost shape `(x_dim, y_dim)`.
- **mvn** (*MultivariateNormal*) – A multivariate normal distribution.

Returns A Gaussian with broadcasted batch shape and `.dim() == x_dim + y_dim`.

Return type *Gaussian*

gaussian_tensordot(*x*, *y*, *dims=0*)

Computes the integral over two gaussians:

(x @ y)(a,c) = log(integral(exp(x(a,b) + y(b,c)), b)),

where *x* is a gaussian over variables (a,b), *y* is a gaussian over variables (b,c), (a,b,c) can each be sets of zero or more variables, and *dims* is the size of b.

Parameters

- **x** – a Gaussian instance
- **y** – a Gaussian instance
- **dims** – number of variables to contract

9.8 Statistical Utilities

gelman_rubin(*input*, *chain_dim=0*, *sample_dim=1*)

Computes R-hat over chains of samples. It is required that `input.size(sample_dim) >= 2` and `input.size(chain_dim) >= 2`.

Parameters

- **input** (*torch.Tensor*) – the input tensor.
- **chain_dim** (*int*) – the chain dimension.
- **sample_dim** (*int*) – the sample dimension.

Returns torch.Tensor R-hat of `input`.

split_gelman_rubin(*input*, *chain_dim=0*, *sample_dim=1*)

Computes R-hat over chains of samples. It is required that `input.size(sample_dim) >= 4`.

Parameters

- **input** (*torch.Tensor*) – the input tensor.
- **chain_dim** (*int*) – the chain dimension.
- **sample_dim** (*int*) – the sample dimension.

Returns torch.Tensor split R-hat of `input`.

autocorrelation(*input*, *dim=0*)

Computes the autocorrelation of samples at dimension `dim`.

Reference: https://en.wikipedia.org/wiki/Autocorrelation#Efficient_computation

Parameters

- **input** (*torch.Tensor*) – the input tensor.
- **dim** (*int*) – the dimension to calculate autocorrelation.

Returns torch.Tensor autocorrelation of `input`.

autocovariance(*input*, *dim=0*)
Computes the autocovariance of samples at dimension `dim`.

Parameters

- **input** (*torch.Tensor*) – the input tensor.
- **dim** (*int*) – the dimension to calculate autocorrelation.

Returns torch.Tensor autocorrelation of `input`.

effective_sample_size(*input*, *chain_dim=0*, *sample_dim=1*)
Computes effective sample size of input.

Reference:

[1] ***Introduction to Markov Chain Monte Carlo*****,** Charles J. Geyer

[2] ***Stan Reference Manual version 2.18*****,** Stan Development Team

Parameters

- **input** (*torch.Tensor*) – the input tensor.
- **chain_dim** (*int*) – the chain dimension.
- **sample_dim** (*int*) – the sample dimension.

Returns torch.Tensor effective sample size of `input`.

resample(*input*, *num_samples*, *dim=0*, *replacement=False*)
Draws `num_samples` samples from `input` at dimension `dim`.

Parameters

- **input** (*torch.Tensor*) – the input tensor.
- **num_samples** (*int*) – the number of samples to draw from `input`.
- **dim** (*int*) – dimension to draw from `input`.

Returns torch.Tensor samples drawn randomly from `input`.

quantile(*input*, *probs*, *dim=0*)
Computes quantiles of `input` at `probs`. If `probs` is a scalar, the output will be squeezed at `dim`.

Parameters

- **input** (*torch.Tensor*) – the input tensor.
- **probs** (*list*) – quantile positions.
- **dim** (*int*) – dimension to take quantiles from `input`.

Returns torch.Tensor quantiles of `input` at `probs`.

pi(*input*, *prob*, *dim=0*)
Computes percentile interval which assigns equal probability mass to each tail of the interval.

Parameters

- **input** (*torch.Tensor*) – the input tensor.
- **prob** (*float*) – the probability mass of samples within the interval.
- **dim** (*int*) – dimension to calculate percentile interval from `input`.

Returns torch.Tensor quantiles of `input` at `probs`.

hpdi (*input*, *prob*, *dim=0*)
Computes "highest posterior density interval" which is the narrowest interval with probability mass `prob`.

Parameters

- **input** (*torch.Tensor*) – the input tensor.
- **prob** (*float*) – the probability mass of samples within the interval.
- **dim** (*int*) – dimension to calculate percentile interval from `input`.

Returns torch.Tensor quantiles of `input` at `probs`.

waic (*input*, *log_weights=None*, *pointwise=False*, *dim=0*)
Computes "Widely Applicable/Watanabe-Akaike Information Criterion" (WAIC) and its corresponding effective number of parameters.

Reference:

[1] *WAIC and cross-validation in Stan*, Aki Vehtari, Andrew Gelman

Parameters

- **input** (*torch.Tensor*) – the input tensor, which is log likelihood of a model.
- **log_weights** (*torch.Tensor*) – weights of samples along `dim`.
- **dim** (*int*) – the sample dimension of `input`.

Returns tuple tuple of WAIC and effective number of parameters.

fit_generalized_pareto (*X*)
Given a dataset X assumed to be drawn from the Generalized Pareto Distribution, estimate the distributional parameters k, sigma using a variant of the technique described in reference [1], as described in reference [2].

References [1] 'A new and efficient estimation method for the generalized Pareto distribution.' Zhang, J. and Stephens, M.A. (2009). [2] 'Pareto Smoothed Importance Sampling.' Aki Vehtari, Andrew Gelman, Jonah Gabry

Parameters **torch.Tensor** – the input data X

Returns tuple tuple of floats (k, sigma) corresponding to the fit parameters

crps_empirical (*pred*, *truth*)
Computes negative Continuous Ranked Probability Score CRPS* [1] between a set of samples `pred` and true data `truth`. This uses an `n log(n)` time algorithm to compute a quantity equal that would naively have complexity quadratic in the number of samples `n`:

```
CRPS* = E|pred - truth| - 1/2 E|pred - pred'|
      = (pred - truth).abs().mean(0)
      - (pred - pred.unsqueeze(1)).abs().mean([0, 1]) / 2
```

Note that for a single sample this reduces to absolute error.

References

[1] Tilmann Gneiting, Adrian E. Raftery (2007) *Strictly Proper Scoring Rules, Prediction, and Estimation* https://www.stat.washington.edu/raftery/Research/PDF/Gneiting2007jasa.pdf

Parameters

- **pred** (*torch.Tensor*) – A set of sample predictions batched on rightmost dim. This should have shape `(num_samples,) + truth.shape`.
- **truth** (*torch.Tensor*) – A tensor of true observations.

Returns A tensor of shape `truth.shape`.

Return type torch.Tensor

9.9 State Space Model and GP Utilities

class MaternKernel(*nu=1.5*, *num_gps=1*, *length_scale_init=None*, *kernel_scale_init=None*)
Bases: *pyro.nn.module.PyroModule*

Provides the building blocks for representing univariate Gaussian Processes (GPs) with Matern kernels as state space models.

Parameters

- **nu** (*float*) – The order of the Matern kernel (one of 0.5, 1.5 or 2.5)
- **num_gps** (*int*) – the number of GPs
- **length_scale_init** (*torch.Tensor*) – optional *num_gps*-dimensional vector of initializers for the length scale
- **kernel_scale_init** (*torch.Tensor*) – optional *num_gps*-dimensional vector of initializers for the kernel scale

References

[1] ***Kalman Filtering and Smoothing Solutions to Temporal Gaussian Process Regression Models***, Jouni Hartikainen and Simo Sarkka.

[2] ***Stochastic Differential Equation Methods for Spatio-Temporal Gaussian Process Regression***, Arno Solin.

transition_matrix(*dt*)
Compute the (exponentiated) transition matrix of the GP latent space. The resulting matrix has layout (num_gps, old_state, new_state), i.e. this matrix multiplies states from the right.

See section 5 in reference [1] for details.

Parameters **dt** (*float*) – the time interval over which the GP latent space evolves.

Returns torch.Tensor a 3-dimensional tensor of transition matrices of shape (num_gps, state_dim, state_dim).

stationary_covariance()
Compute the stationary state covariance. See Eqn. 3.26 in reference [2].

Returns torch.Tensor a 3-dimensional tensor of covariance matrices of shape (num_gps, state_dim, state_dim).

process_covariance(*A*)
Given a transition matrix *A* computed with *transition_matrix* compute the the process covariance as described in Eqn. 3.11 in reference [2].

Returns torch.Tensor a batched covariance matrix of shape (num_gps, state_dim, state_dim)

transition_matrix_and_covariance(*dt*)
Get the transition matrix and process covariance corresponding to a time interval *dt*.

Parameters **dt** (*float*) – the time interval over which the GP latent space evolves.

Returns tuple (*transition_matrix*, *process_covariance*) both 3-dimensional tensors of shape (num_gps, state_dim, state_dim)

CHAPTER 10

Automatic Name Generation

The *pyro.contrib.autoname* module provides tools for automatically generating unique, semantically meaningful names for sample sites.

scope (*fn=None*, *prefix=None*, *inner=None*)

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls)
- **prefix** – a string to prepend to sample names (optional if `fn` is provided)
- **inner** – switch to determine where duplicate name counters appear

Returns `fn` decorated with a *ScopeMessenger*

`scope` prepends a prefix followed by a `/` to the name at a Pyro sample site. It works much like TensorFlow's `name_scope` and `variable_scope`, and can be used as a context manager, a decorator, or a higher-order function.

`scope` is very useful for aligning compositional models with guides or data.

Example:

```
>>> @scope(prefix="a")
... def model():
...     return pyro.sample("x", dist.Bernoulli(0.5))
...
>>> assert "a/x" in poutine.trace(model).get_trace()
```

Example:

```
>>> def model():
...     with scope(prefix="a"):
...         return pyro.sample("x", dist.Bernoulli(0.5))
...
>>> assert "a/x" in poutine.trace(model).get_trace()
```

Scopes compose as expected, with outer scopes appearing before inner scopes in names:

```
>>> @scope(prefix="b")
... def model():
...     with scope(prefix="a"):
...         return pyro.sample("x", dist.Bernoulli(0.5))
...
>>> assert "b/a/x" in poutine.trace(model).get_trace()
```

When used as a decorator or higher-order function, `scope` will use the name of the input function as the prefix if no user-specified prefix is provided.

Example:

```
>>> @scope
... def model():
...     return pyro.sample("x", dist.Bernoulli(0.5))
...
>>> assert "model/x" in poutine.trace(model).get_trace()
```

name_count (*fn=None*)

`name_count` is a very simple autonaming scheme that simply appends a suffix "__" plus a counter to any name that appears multiple tims in an execution. Only duplicate instances of a name get a suffix; the first instance is not modified.

Example:

```
>>> @name_count
... def model():
...     for i in range(3):
...         pyro.sample("x", dist.Bernoulli(0.5))
...
>>> assert "x" in poutine.trace(model).get_trace()
>>> assert "x__1" in poutine.trace(model).get_trace()
>>> assert "x__2" in poutine.trace(model).get_trace()
```

`name_count` also composes with *`scope()`* by adding a suffix to duplicate scope entrances:

Example:

```
>>> @name_count
... def model():
...     for i in range(3):
...         with pyro.contrib.autoname.scope(prefix="a"):
...             pyro.sample("x", dist.Bernoulli(0.5))
...
>>> assert "a/x" in poutine.trace(model).get_trace()
>>> assert "a__1/x" in poutine.trace(model).get_trace()
>>> assert "a__2/x" in poutine.trace(model).get_trace()
```

Example:

```
>>> @name_count
... def model():
...     with pyro.contrib.autoname.scope(prefix="a"):
...         for i in range(3):
...             pyro.sample("x", dist.Bernoulli(0.5))
...
>>> assert "a/x" in poutine.trace(model).get_trace()
```

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```
>>> assert "a/x__1" in poutine.trace(model).get_trace()
>>> assert "a/x__2" in poutine.trace(model).get_trace()
```

10.1 Named Data Structures

The `pyro.contrib.named` module is a thin syntactic layer on top of Pyro. It allows Pyro models to be written to look like programs with operating on Python data structures like `latent.x.sample_(...)`, rather than programs with string-labeled statements like `x = pyro.sample("x", ...)`.

This module provides three container data structures `named.Object`, `named.List`, and `named.Dict`. These data structures are intended to be nested in each other. Together they track the address of each piece of data in each data structure, so that this address can be used as a Pyro site. For example:

```
>>> state = named.Object("state")
>>> print(str(state))
state

>>> z = state.x.y.z  # z is just a placeholder.
>>> print(str(z))
state.x.y.z

>>> state.xs = named.List()  # Create a contained list.
>>> x0 = state.xs.add()
>>> print(str(x0))
state.xs[0]

>>> state.ys = named.Dict()
>>> foo = state.ys['foo']
>>> print(str(foo))
state.ys['foo']
```

These addresses can now be used inside `sample`, `observe` and `param` statements. These named data structures even provide in-place methods that alias Pyro statements. For example:

```
>>> state = named.Object("state")
>>> loc = state.loc.param_(torch.zeros(1, requires_grad=True))
>>> scale = state.scale.param_(torch.ones(1, requires_grad=True))
>>> z = state.z.sample_(dist.Normal(loc, scale))
>>> obs = state.x.sample_(dist.Normal(loc, scale), obs=z)
```

For deeper examples of how these can be used in model code, see the Tree Data and Mixture examples.

Authors: Fritz Obermeyer, Alexander Rush

class Object(*name*)

Bases: `object`

Object to hold immutable latent state.

This object can serve either as a container for nested latent state or as a placeholder to be replaced by a tensor via a named.sample, named.observe, or named.param statement. When used as a placeholder, Object objects take the place of strings in normal pyro.sample statements.

Parameters **name** (*str*) – The name of the object.

Example:

```
state = named.Object("state")
state.x = 0
state.ys = named.List()
state.zs = named.Dict()
state.a.b.c.d.e.f.g = 0  # Creates a chain of named.Objects.
```

Warning: This data structure is write-once: data may be added but may not be mutated or removed. Trying to mutate this data structure may result in silent errors.

sample_(*fn*, **args*, ***kwargs*)

Calls the stochastic function *fn* with additional side-effects depending on *name* and the enclosing context (e.g. an inference algorithm). See Intro I and Intro II for a discussion.

Parameters

- **name** – name of sample
- **fn** – distribution class or function
- **obs** – observed datum (optional; should only be used in context of inference) optionally specified in kwargs
- **infer** (*dict*) – Optional dictionary of inference parameters specified in kwargs. See inference documentation for details.

Returns sample

param_(**args*, ***kwargs*)

Saves the variable as a parameter in the param store. To interact with the param store or write to disk, see Parameters.

Parameters

- **name** (*str*) – name of parameter
- **init_tensor** (*torch.Tensor or callable*) – initial tensor or lazy callable that returns a tensor. For large tensors, it may be cheaper to write e.g. `lambda: torch.randn(100000)`, which will only be evaluated on the initial statement.
- **constraint** (*torch.distributions.constraints.Constraint*) – torch constraint, defaults to `constraints.real`.
- **event_dim** (*int*) – (optional) number of rightmost dimensions unrelated to baching. Dimension to the left of this will be considered batch dimensions; if the param statement is inside a subsampled plate, then corresponding batch dimensions of the parameter will be correspondingly subsampled. If unspecified, all dimensions will be considered event dims and no subsampling will be performed.

Returns parameter

Return type torch.Tensor

class List(*name=None*)

Bases: `list`

List-like object to hold immutable latent state.

This must either be given a name when constructed:

```
latent = named.List("root")
```

or must be immediately stored in a `named.Object`:

```
latent = named.Object("root")
latent.xs = named.List()  # Must be bound to a Object before use.
```

Warning: This data structure is write-once: data may be added but may not be mutated or removed. Trying to mutate this data structure may result in silent errors.

add()
Append one new named.Object.

Returns a new latent object at the end

Return type *named.Object*

class Dict(*name=None*)
Bases: `dict`

Dict-like object to hold immutable latent state.

This must either be given a name when constructed:

```
latent = named.Dict("root")
```

or must be immediately stored in a `named.Object`:

```
latent = named.Object("root")
latent.xs = named.Dict()  # Must be bound to a Object before use.
```

Warning: This data structure is write-once: data may be added but may not be mutated or removed. Trying to mutate this data structure may result in silent errors.

10.2 Scoping

`pyro.contrib.autoname.scoping` contains the implementation of *pyro.contrib.autoname.scope()*, a tool for automatically appending a semantically meaningful prefix to names of sample sites.

class NameCountMessenger
Bases: *pyro.poutine.messenger.Messenger*

`NameCountMessenger` is the implementation of *pyro.contrib.autoname.name_count()*

class ScopeMessenger(*prefix=None*, *inner=None*)
Bases: *pyro.poutine.messenger.Messenger*

`ScopeMessenger` is the implementation of *pyro.contrib.autoname.scope()*

scope(*fn=None*, *prefix=None*, *inner=None*)

Parameters

- **fn** – a stochastic function (callable containing Pyro primitive calls)

- **prefix** – a string to prepend to sample names (optional if `fn` is provided)
- **inner** – switch to determine where duplicate name counters appear

Returns `fn` decorated with a *ScopeMessenger*

`scope` prepends a prefix followed by a `/` to the name at a Pyro sample site. It works much like TensorFlow's `name_scope` and `variable_scope`, and can be used as a context manager, a decorator, or a higher-order function.

`scope` is very useful for aligning compositional models with guides or data.

Example:

```
>>> @scope(prefix="a")
... def model():
...     return pyro.sample("x", dist.Bernoulli(0.5))
...
>>> assert "a/x" in poutine.trace(model).get_trace()
```

Example:

```
>>> def model():
...     with scope(prefix="a"):
...         return pyro.sample("x", dist.Bernoulli(0.5))
...
>>> assert "a/x" in poutine.trace(model).get_trace()
```

Scopes compose as expected, with outer scopes appearing before inner scopes in names:

```
>>> @scope(prefix="b")
... def model():
...     with scope(prefix="a"):
...         return pyro.sample("x", dist.Bernoulli(0.5))
...
>>> assert "b/a/x" in poutine.trace(model).get_trace()
```

When used as a decorator or higher-order function, `scope` will use the name of the input function as the prefix if no user-specified prefix is provided.

Example:

```
>>> @scope
... def model():
...     return pyro.sample("x", dist.Bernoulli(0.5))
...
>>> assert "model/x" in poutine.trace(model).get_trace()
```

name_count (*fn=None*)

`name_count` is a very simple autonaming scheme that simply appends a suffix "__" plus a counter to any name that appears multiple tims in an execution. Only duplicate instances of a name get a suffix; the first instance is not modified.

Example:

```
>>> @name_count
... def model():
...     for i in range(3):
...         pyro.sample("x", dist.Bernoulli(0.5))
...
```

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```
>>> assert "x" in poutine.trace(model).get_trace()
>>> assert "x__1" in poutine.trace(model).get_trace()
>>> assert "x__2" in poutine.trace(model).get_trace()
```

`name_count` also composes with *`scope()`* by adding a suffix to duplicate scope entrances:

Example:

```
>>> @name_count
... def model():
...     for i in range(3):
...         with pyro.contrib.autoname.scope(prefix="a"):
...             pyro.sample("x", dist.Bernoulli(0.5))
...
>>> assert "a/x" in poutine.trace(model).get_trace()
>>> assert "a__1/x" in poutine.trace(model).get_trace()
>>> assert "a__2/x" in poutine.trace(model).get_trace()
```

Example:

```
>>> @name_count
... def model():
...     with pyro.contrib.autoname.scope(prefix="a"):
...         for i in range(3):
...             pyro.sample("x", dist.Bernoulli(0.5))
...
>>> assert "a/x" in poutine.trace(model).get_trace()
>>> assert "a/x__1" in poutine.trace(model).get_trace()
>>> assert "a/x__2" in poutine.trace(model).get_trace()
```

CHAPTER 11

Bayesian Neural Networks

11.1 HiddenLayer

class HiddenLayer(*X=None*, *A_mean=None*, *A_scale=None*, *non_linearity=<function relu>*, *KL_factor=1.0*, *A_prior_scale=1.0*, *include_hidden_bias=True*, *weight_space_sampling=False*)

This distribution is a basic building block in a Bayesian neural network. It represents a single hidden layer, i.e. an affine transformation applied to a set of inputs *X* followed by a non-linearity. The uncertainty in the weights is encoded in a Normal variational distribution specified by the parameters *A_scale* and *A_mean*. The so-called 'local reparameterization trick' is used to reduce variance (see reference below). In effect, this means the weights are never sampled directly; instead one samples in pre-activation space (i.e. before the non-linearity is applied). Since the weights are never directly sampled, when this distribution is used within the context of variational inference, care must be taken to correctly scale the KL divergence term that corresponds to the weight matrix. This term is folded into the *log_prob* method of this distributions.

In effect, this distribution encodes the following generative process:

A ~ Normal(A_mean, A_scale) output ~ non_linearity(AX)

Parameters

- **X** (*torch.Tensor*) – B x D dimensional mini-batch of inputs
- **A_mean** (*torch.Tensor*) – D x H dimensional specifiying weight mean
- **A_scale** (*torch.Tensor*) – D x H dimensional (diagonal covariance matrix) specifying weight uncertainty
- **non_linearity** (*callable*) – a callable that specifies the non-linearity used. defaults to ReLU.
- **KL_factor** (*float*) – scaling factor for the KL divergence. prototypically this is equal to the size of the mini-batch divided by the size of the whole dataset. defaults to *1.0*.
- **A_prior** (*float or torch.Tensor*) – the prior over the weights is assumed to be normal with mean zero and scale factor *A_prior*. default value is 1.0.

- **include_hidden_bias** (*bool*) – controls whether the activations should be augmented with a 1, which can be used to incorporate bias terms. defaults to *True*.
- **weight_space_sampling** (*bool*) – controls whether the local reparameterization trick is used. this is only intended to be used for internal testing. defaults to *False*.

Reference:

Kingma, Diederik P., Tim Salimans, and Max Welling. "Variational dropout and the local reparameterization trick." Advances in Neural Information Processing Systems. 2015.

CHAPTER 12

Causal Effect VAE

This module implements the Causal Effect Variational Autoencoder [1], which demonstrates a number of innovations including:

- a generative model for causal effect inference with hidden confounders;
- a model and guide with twin neural nets to allow imbalanced treatment; and
- a custom training loss that includes both ELBO terms and extra terms needed to train the guide to be able to answer counterfactual queries.

The main interface is the *CEVAE* class, but users may customize by using components *Model*, *Guide*, *TraceCausalEffect_ELBO* and utilities.

References

[1] C. Louizos, U. Shalit, J. Mooij, D. Sontag, R. Zemel, M. Welling (2017).

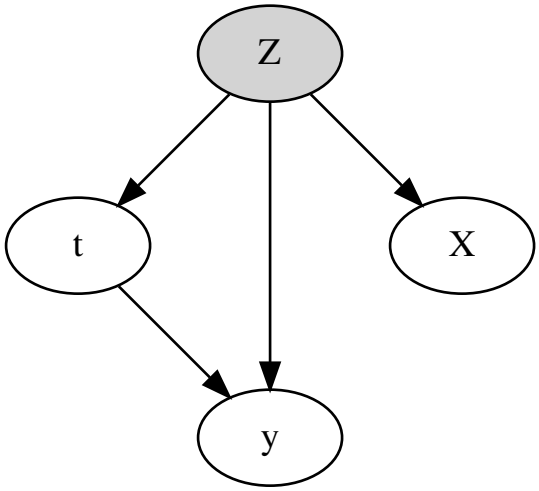
Causal Effect Inference with Deep Latent-Variable Models.
http://papers.nips.cc/paper/7223-causal-effect-inference-with-deep-latent-variable-models.pdf
https://github.com/AMLab-Amsterdam/CEVAE

12.1 CEVAE Class

class CEVAE(*feature_dim*, *outcome_dist='bernoulli'*, *latent_dim=20*, *hidden_dim=200*, *num_layers=3*, *num_samples=100*)

Bases: `torch.nn.modules.module.Module`

Main class implementing a Causal Effect VAE [1]. This assumes a graphical model



where t is a binary treatment variable, y is an outcome, Z is an unobserved confounder, and X is a noisy function of the hidden confounder Z.

Example:

```
cevae = CEVAE(feature_dim=5)
cevae.fit(x_train, t_train, y_train)
ite = cevae.ite(x_test)  # individual treatment effect
ate = ite.mean()         # average treatment effect
```

Variables

- **model** (Model) – Generative model.
- **guide** (Guide) – Inference model.

Parameters

- **feature_dim** (*int*) – Dimension of the feature space x.
- **outcome_dist** (*str*) – One of: "bernoulli" (default), "exponential", "laplace", "normal", "studentt".
- **latent_dim** (*int*) – Dimension of the latent variable z. Defaults to 20.
- **hidden_dim** (*int*) – Dimension of hidden layers of fully connected networks. Defaults to 200.
- **num_layers** (*int*) – Number of hidden layers in fully connected networks.
- **num_samples** (*int*) – Default number of samples for the *ite()* method. Defaults to 100.

fit(*x*, *t*, *y*, *num_epochs=100*, *batch_size=100*, *learning_rate=0.001*, *learning_rate_decay=0.1*, *weight_decay=0.0001*)

Train using *SVI* with the *TraceCausalEffect_ELBO* loss.

Parameters

- **x** (*Tensor*) –
- **t** (*Tensor*) –
- **y** (*Tensor*) –
- **num_epochs** (*int*) – Number of training epochs. Defaults to 100.
- **batch_size** (*int*) – Batch size. Defaults to 100.
- **learning_rate** (*float*) – Learning rate. Defaults to 1e-3.
- **learning_rate_decay** (*float*) – Learning rate decay over all epochs; the per-step decay rate will depend on batch size and number of epochs such that the initial learning rate will be `learning_rate` and the final learning rate will be `learning_rate * learning_rate_decay`. Defaults to 0.1.
- **weight_decay** (*float*) – Weight decay. Defaults to 1e-4.

Returns list of epoch losses

ite(*x*, *num_samples=None*, *batch_size=None*)

Computes Individual Treatment Effect for a batch of data `x`.

$$ITE(x) = \mathbb{E}\big[\mathbf{y} \mid \mathbf{X} = x, do(\mathbf{t} = 1)\big] - \mathbb{E}\big[\mathbf{y} \mid \mathbf{X} = x, do(\mathbf{t} = 0)\big]$$

This has complexity `O(len(x) * num_samples ** 2)`.

Parameters

- **x** (*Tensor*) – A batch of data.
- **num_samples** (*int*) – The number of monte carlo samples. Defaults to `self.num_samples` which defaults to `100`.
- **batch_size** (*int*) – Batch size. Defaults to `len(x)`.

Returns A `len(x)`-sized tensor of estimated effects.

Return type Tensor

to_script_module()

Compile this module using `torch.jit.trace_module()` , assuming self has already been fit to data.

Returns A traced version of self with an *ite()* method.

Return type torch.jit.ScriptModule

12.2 CEVAE Components

class Model(*config*)

Bases: *pyro.nn.module.PyroModule*

Generative model for a causal model with latent confounder `z` and binary treatment `t`:

```
z ~ p(z)       # latent confounder
x ~ p(x|z)     # partial noisy observation of z
t ~ p(t|z)     # treatment, whose application is biased by z
y ~ p(y|t,z)   # outcome
```

Each of these distributions is defined by a neural network. The `y` distribution is defined by a disjoint pair of neural networks defining `p(y|t=0,z)` and `p(y|t=1,z)`; this allows highly imbalanced treatment.

Parameters **config** (*dict*) – A dict specifying `feature_dim`, `latent_dim`, `hidden_dim`, `num_layers`, and `outcome_dist`.

forward (*x*, *t=None*, *y=None*, *size=None*)

y_mean (*x*, *t=None*)

z_dist ()

x_dist (*z*)

y_dist (*t*, *z*)

t_dist (*z*)

class Guide (*config*)

Bases: *pyro.nn.module.PyroModule*

Inference model for causal effect estimation with latent confounder `z` and binary treatment `t`:

```
t ~ q(t|x)       # treatment
y ~ q(y|t,x)     # outcome
z ~ q(z|y,t,x)   # latent confounder, an embedding
```

Each of these distributions is defined by a neural network. The `y` and `z` distributions are defined by disjoint pairs of neural networks defining `p(-|t=0,...)` and `p(-|t=1,...)`; this allows highly imbalanced treatment.

Parameters **config** (*dict*) – A dict specifying `feature_dim`, `latent_dim`, `hidden_dim`, `num_layers`, and `outcome_dist`.

forward (*x*, *t=None*, *y=None*, *size=None*)

t_dist (*x*)

y_dist (*t*, *x*)

z_dist (*y*, *t*, *x*)

class TraceCausalEffect_ELBO (*num_particles=1*, *max_plate_nesting=inf*, *max_iarange_nesting=None*, *vectorize_particles=False*, *strict_enumeration_warning=True*, *ignore_jit_warnings=False*, *jit_options=None*, *retain_graph=None*, *tail_adaptive_beta=-1.0*)

Bases: *pyro.infer.trace_elbo.Trace_ELBO*

Loss function for training a *CEVAE*. From [1], the CEVAE objective (to maximize) is:

```
-loss = ELBO + log q(t|x) + log q(y|t,x)
```

loss (*model*, *guide*, **args*, ***kwargs*)

12.3 Utilities

class FullyConnected (*sizes*, *final_activation=None*)

Bases: `torch.nn.modules.container.Sequential`

Fully connected multi-layer network with ELU activations.

append (*layer*)

class DistributionNet
Bases: torch.nn.modules.module.Module

Base class for distribution nets.

static get_class(*dtype*)
Get a subclass by a prefix of its name, e.g.:

```
assert DistributionNet.get_class("bernoulli") is BernoulliNet
```

class BernoulliNet(*sizes*)
Bases: *pyro.contrib.cevae.DistributionNet*

FullyConnected network outputting a single `logits` value.

This is used to represent a conditional probability distribution of a single Bernoulli random variable conditioned on a `sizes[0]`-sized real value, for example:

```
net = BernoulliNet([3, 4])
z = torch.randn(3)
logits, = net(z)
t = net.make_dist(logits).sample()
```

forward(*x*)

static make_dist(*logits*)

class ExponentialNet(*sizes*)
Bases: *pyro.contrib.cevae.DistributionNet*

FullyConnected network outputting a constrained `rate`.

This is used to represent a conditional probability distribution of a single Normal random variable conditioned on a `sizes[0]`-size real value, for example:

```
net = ExponentialNet([3, 4])
x = torch.randn(3)
rate, = net(x)
y = net.make_dist(rate).sample()
```

forward(*x*)

static make_dist(*rate*)

class LaplaceNet(*sizes*)
Bases: *pyro.contrib.cevae.DistributionNet*

FullyConnected network outputting a constrained `loc,scale` pair.

This is used to represent a conditional probability distribution of a single Laplace random variable conditioned on a `sizes[0]`-size real value, for example:

```
net = LaplaceNet([3, 4])
x = torch.randn(3)
loc, scale = net(x)
y = net.make_dist(loc, scale).sample()
```

forward(*x*)

static make_dist(*loc*, *scale*)

class NormalNet(*sizes*)
Bases: *pyro.contrib.cevae.DistributionNet*

FullyConnected network outputting a constrained `loc, scale` pair.

This is used to represent a conditional probability distribution of a single Normal random variable conditioned on a `sizes[0]`-size real value, for example:

```
net = NormalNet([3, 4])
x = torch.randn(3)
loc, scale = net(x)
y = net.make_dist(loc, scale).sample()
```

forward(*x*)

static make_dist(*loc*, *scale*)

class StudentTNet(*sizes*)

Bases: *pyro.contrib.cevae.DistributionNet*

FullyConnected network outputting a constrained `df, loc, scale` triple, with shared `df > 1`.

This is used to represent a conditional probability distribution of a single Student's t random variable conditioned on a `sizes[0]`-size real value, for example:

```
net = StudentTNet([3, 4])
x = torch.randn(3)
df, loc, scale = net(x)
y = net.make_dist(df, loc, scale).sample()
```

forward(*x*)

static make_dist(*df*, *loc*, *scale*)

class DiagNormalNet(*sizes*)

Bases: `torch.nn.modules.module.Module`

FullyConnected network outputting a constrained `loc, scale` pair.

This is used to represent a conditional probability distribution of a `sizes[-1]`-sized diagonal Normal random variable conditioned on a `sizes[0]`-size real value, for example:

```
net = DiagNormalNet([3, 4, 5])
z = torch.randn(3)
loc, scale = net(z)
x = dist.Normal(loc, scale).sample()
```

This is intended for the latent `z` distribution and the prewhitened `x` features, and conservatively clips `loc` and `scale` values.

forward(*x*)

CHAPTER 13

Easy Custom Guides

13.1 EasyGuide

class EasyGuide(*model*)

Bases: *pyro.nn.module.PyroModule*

Base class for "easy guides", which are more flexible than `AutoGuide` s, but are easier to write than raw Pyro guides.

Derived classes should define a *guide()* method. This *guide()* method can combine ordinary guide statements (e.g. `pyro.sample` and `pyro.param`) with the following special statements:

- `group = self.group(...)` selects multiple `pyro.sample` sites in the model. See `Group` for subsequent methods.
- `with self.plate(...): ...` should be used instead of `pyro.plate`.
- `self.map_estimate(...)` uses a `Delta` guide for a single site.

Derived classes may also override the *init()* method to provide custom initialization for models sites.

Parameters **model** (*callable*) – A Pyro model.

model

guide(**args*, ***kargs*)

Guide implementation, to be overridden by user.

init(*site*)

Model initialization method, may be overridden by user.

This should input a site and output a valid sample from that site. The default behavior is to draw a random sample:

```
return site["fn"]()
```

For other possible initialization functions see http://docs.pyro.ai/en/stable/infer.autoguide.html#module-pyro.infer.autoguide.initialization

forward(**args*, ***kwargs*)
Runs the guide. This is typically used by inference algorithms.

Note: This method is used internally by `Module`. Users should instead use `__call__()`.

plate(*name*, *size=None*, *subsample_size=None*, *subsample=None*, **args*, ***kwargs*)
A wrapper around `pyro.plate` to allow *EasyGuide* to automatically construct plates. You should use this rather than `pyro.plate` inside your *guide()* implementation.

group(*match='.*'*)
Select a `Group` of model sites for joint guidance.

Parameters **match** (*str*) – A regex string matching names of model sample sites.

Returns A group of model sites.

Return type *Group*

map_estimate(*name*)
Construct a maximum a posteriori (MAP) guide using Delta distributions.

Parameters **name** (*str*) – The name of a model sample site.

Returns A sampled value.

Return type torch.Tensor

13.2 easy_guide

easy_guide(*model*)
Convenience decorator to create an *EasyGuide* . The following are equivalent:

```
# Version 1. Decorate a function.
@easy_guide(model)
def guide(self, foo, bar):
    return my_guide(foo, bar)

# Version 2. Create and instantiate a subclass of EasyGuide.
class Guide(EasyGuide):
    def guide(self, foo, bar):
        return my_guide(foo, bar)
guide = Guide(model)
```

Note `@easy_guide` wrappers cannot be pickled; to build a guide that can be pickled, instead subclass from *EasyGuide*.

Parameters **model** (*callable*) – a Pyro model.

13.3 Group

class Group(*guide*, *sites*)
Bases: `object`

An autoguide helper to match a group of model sites.

Variables

- ***event_shape*** (*torch.Size*) – The total flattened concatenated shape of all matching sample sites in the model.
- **prototype_sites** (*list*) – A list of all matching sample sites in a prototype trace of the model.

Parameters

- **guide** (EasyGuide) – An easyguide instance.
- **sites** (*list*) – A list of model sites.

guide

sample(*guide_name*, *fn*, *infer=None*)

Wrapper around `pyro.sample()` to create a single auxiliary sample site and then unpack to multiple sample sites for model replay.

Parameters

- **guide_name** (*str*) – The name of the auxiliary guide site.
- **fn** (*callable*) – A distribution with shape `self.event_shape`.
- **infer** (*dict*) – Optional inference configuration dict.

Returns A pair `(guide_z, model_zs)` where `guide_z` is the single concatenated blob and `model_zs` is a dict mapping site name to constrained model sample.

Return type tuple

map_estimate()

Construct a maximum a posteriori (MAP) guide using Delta distributions.

Returns A dict mapping model site name to sampled value.

Return type dict

CHAPTER 14

Epidemiology

Warning: Code in `pyro.contrib.epidemiology` is under development. This code makes no guarantee about maintaining backwards compatibility.

`pyro.contrib.epidemiology` provides a modeling language for a class of stochastic discrete-time discrete-count compartmental models. This module implements black-box **inference** (both Stochastic Variational Inference and Hamiltonian Monte Carlo), **prediction** of latent variables, and **forecasting** of future trajectories.

For example usage see the following tutorials:

- Introduction
- Univariate models
- Regional models
- Inference via auxiliary variable HMC

14.1 Base Compartmental Model

class CompartmentalModel(*compartments*, *duration*, *population*, *, *approximate=()*)

Bases: `abc.ABC`

Abstract base class for discrete-time discrete-value stochastic compartmental models.

Derived classes must implement methods *initialize()* and *transition()*. Derived classes may optionally implement *global_model()*, *compute_flows()*, and *heuristic()*.

Example usage:

```
# First implement a concrete derived class.
class MyModel(CompartmentalModel):
    def __init__(self, ...): ...
```

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```
    def global_model(self): ...
    def initialize(self, params): ...
    def transition(self, params, state, t): ...

# Run inference to fit the model to data.
model = MyModel(...)
model.fit_svi(num_samples=100)  # or .fit_mcmc(...)
R0 = model.samples["R0"]  # An example parameter.
print("R0 = {:0.3g} ± {:0.3g}".format(R0.mean(), R0.std()))

# Predict latent variables.
samples = model.predict()

# Forecast forward.
samples = model.predict(forecast=30)

# You can assess future interventions (applied after ``duration``) by
# storing them as attributes that are read by your derived methods.
model.my_intervention = False
samples1 = model.predict(forecast=30)
model.my_intervention = True
samples2 = model.predict(forecast=30)
effect = samples2["my_result"].mean() - samples1["my_result"].mean()
print("average effect = {:0.3g}".format(effect))
```

An example workflow is to use cheaper approximate inference while finding good model structure and priors, then move to more accurate but more expensive inference once the model is plausible.

1. Start with `.fit_svi(guide_rank=0, num_steps=2000)` for cheap inference while you search for a good model.
2. Additionally infer long-range correlations by moving to a low-rank multivariate normal guide via `.fit_svi(guide_rank=None, num_steps=5000)`.
3. Optionally additionally infer non-Gaussian posterior by moving to the more expensive (but still approximate via moment matching) `.fit_mcmc(num_quant_bins=1, num_samples=10000, num_chains=2)`.
4. Optionally improve fit around small counts by moving the the more expensive enumeration-based algorithm `.fit_mcmc(num_quant_bins=4, num_samples=10000, num_chains=2)` (GPU recommended).

Variables **`samples`** (*dict*) – Dictionary of posterior samples.

Parameters

- **`compartments`** (*list*) – A list of strings of compartment names.
- **`duration`** (*int*) – The number of discrete time steps in this model.
- **`population`** (*int or torch.Tensor*) – Either the total population of a single-region model or a tensor of each region's population in a regional model.
- **`approximate`** (*tuple*) – Names of compartments for which pointwise approximations should be provided in *`transition()`*, e.g. if you specify `approximate=("I")` then the `state["I_approx"]` will be a continuous-valued non-enumerated point estimate of `state["I"]`. Approximations are useful to reduce computational cost. Approximations are continuous-valued with support `(-0.5, population + 0.5)`.

time_plate
A `pyro.plate` for the time dimension.

region_plate
Either a `pyro.plate` or a trivial `ExitStack` depending on whether this model `.is_regional`.

full_mass
A list of a single tuple of the names of global random variables.

series
A frozenset of names of sample sites that are sampled each time step.

global_model()
Samples and returns any global parameters.

Returns An arbitrary object of parameters (e.g. `None` or a tuple).

initialize(*params*)
Returns initial counts in each compartment.

Parameters **params** – The global params returned by *global_model()*.

Returns A dict mapping compartment name to initial value.

Return type dict

transition(*params*, *state*, *t*)
Forward generative process for dynamics.

This inputs a current `state` and stochastically updates that state in-place.

Note that this method is called under multiple different interpretations, including batched and vectorized interpretations. During *generate()* this is called to generate a single sample. During *heuristic()* this is called to generate a batch of samples for SMC. During *fit_mcmc()* this is called both in vectorized form (vectorizing over time) and in sequential form (for a single time step); both forms enumerate over discrete latent variables. During *predict()* this is called to forecast a batch of samples, conditioned on posterior samples for the time interval `[0:duration]`.

Parameters

- **params** – The global params returned by *global_model()*.
- **state** (*dict*) – A dictionary mapping compartment name to current tensor value. This should be updated in-place.
- **t** (*int or slice*) – A time-like index. During inference `t` may be either a slice (for vectorized inference) or an integer time index. During prediction `t` will be integer time index.

finalize(*params*, *prev*, *curr*)
Optional method for likelihoods that depend on entire time series.

This should be used only for non-factorizable likelihoods that couple states across time. Factorizable likelihoods should instead be added to the *transition()* method, thereby enabling their use in *heuristic()* initialization. Since this method is called only after the last time step, it is not used in *heuristic()* initialization.

Warning: This currently does not support latent variables.

Parameters

- **params** – The global params returned by *global_model()*.

- **prev** (*dict*) –
- **curr** (*dict*) – Dictionaries mapping compartment name to tensor of entire time series. These two parameters are offset by 1 step, thereby making it easy to compute time series of fluxes. For quantized inference, this uses the approximate point estimates, so users must request any needed time series in `__init__()`, e.g. by calling `super().__init__(..., approximate=("I", "E"))` if likelihood depends on the `I` and `E` time series.

compute_flows (*prev*, *curr*, *t*)

Computes flows between compartments, given compartment populations before and after time step t.

The default implementation assumes sequential flows terminating in an implicit compartment named "R". For example if:

```
compartment_names = ("S", "E", "I")
```

the default implementation computes at time step `t = 9`:

```
flows["S2E_9"] = prev["S"] - curr["S"]
flows["E2I_9"] = prev["E"] - curr["E"] + flows["S2E_9"]
flows["I2R_9"] = prev["I"] - curr["I"] + flows["E2I_9"]
```

For more complex flows (non-sequential, branching, looping, duplicating, etc.), users may override this method.

Parameters

- **state** (*dict*) – A dictionary mapping compartment name to current tensor value. This should be updated in-place.
- **t** (*int or slice*) – A time-like index. During inference `t` may be either a slice (for vectorized inference) or an integer time index. During prediction `t` will be integer time index.

Returns A dict mapping flow name to tensor value.

Return type dict

generate (*fixed={}*)

Generate data from the prior.

Pram dict fixed A dictionary of parameters on which to condition. These must be top-level parentless nodes, i.e. have no upstream stochastic dependencies.

Returns A dictionary mapping sample site name to sampled value.

Return type dict

fit_svi (**, num_samples=100, num_steps=2000, num_particles=32, learning_rate=0.1, learning_rate_decay=0.01, betas=(0.8, 0.99), haar=True, init_scale=0.01, guide_rank=0, jit=False, log_every=200, **options*)

Runs stochastic variational inference to generate posterior samples.

This runs *SVI*, setting the `.samples` attribute on completion.

This approximate inference method is useful for quickly iterating on probabilistic models.

Parameters

- **num_samples** (*int*) – Number of posterior samples to draw from the trained guide. Defaults to 100.

- **num_steps** (*int*) – Number of *SVI* steps.
- **num_particles** (*int*) – Number of *SVI* particles per step.
- **learning_rate** (*int*) – Learning rate for the *ClippedAdam* optimizer.
- **learning_rate_decay** (*int*) – Learning rate for the *ClippedAdam* optimizer. Note this is decay over the entire schedule, not per-step decay.
- **betas** (*tuple*) – Momentum parameters for the *ClippedAdam* optimizer.
- **haar** (*bool*) – Whether to use a Haar wavelet reparameterizer.
- **guide_rank** (*int*) – Rank of the auto normal guide. If zero (default) use an *AutoNormal* guide. If a positive integer or None, use an *AutoLowRankMultivariateNormal* guide. If the string "full", use an *AutoMultivariateNormal* guide. These latter two require more `num_steps` to fit.
- **init_scale** (*float*) – Initial scale of the *AutoLowRankMultivariateNormal* guide.
- **jit** (*bool*) – Whether to use a jit compiled ELBO.
- **log_every** (*int*) – How often to log svi losses.
- **heuristic_num_particles** (*int*) – Passed to *heuristic()* as `num_particles`. Defaults to 1024.

Returns Time series of SVI losses (useful to diagnose convergence).

Return type list

fit_mcmc(***options*)

Runs NUTS inference to generate posterior samples.

This uses the `NUTS` kernel to run *MCMC*, setting the `.samples` attribute on completion.

This uses an asymptotically exact enumeration-based model when `num_quant_bins > 1`, and a cheaper moment-matched approximate model when `num_quant_bins == 1`.

Parameters

- ****options** – Options passed to *MCMC*. The remaining options are pulled out and have special meaning.
- **num_samples** (*int*) – Number of posterior samples to draw via mcmc. Defaults to 100.
- **max_tree_depth** (*int*) – (Default 5). Max tree depth of the `NUTS` kernel.
- **full_mass** – Specification of mass matrix of the `NUTS` kernel. Defaults to full mass over global random variables.
- **arrowhead_mass** (*bool*) – Whether to treat `full_mass` as the head of an arrowhead matrix versus simply as a block. Defaults to False.
- **num_quant_bins** (*int*) – If greater than 1, use asymptotically exact inference via local enumeration over this many quantization bins. If equal to 1, use continuous-valued relaxed approximate inference. Note that computational cost is exponential in *num_quant_bins*. Defaults to 1 for relaxed inference.
- **haar** (*bool*) – Whether to use a Haar wavelet reparameterizer. Defaults to True.
- **haar_full_mass** (*int*) – Number of low frequency Haar components to include in the full mass matrix. If `haar=False` then this is ignored. Defaults to 10.

- **heuristic_num_particles** (*int*) – Passed to *heuristic()* as `num_particles`. Defaults to 1024.

Returns An MCMC object for diagnostics, e.g. `MCMC.summary()`.

Return type *MCMC*

predict (*forecast=0*)

Predict latent variables and optionally forecast forward.

This may be run only after *fit_mcmc()* and draws the same `num_samples` as passed to *fit_mcmc()*.

Parameters **forecast** (*int*) – The number of time steps to forecast forward.

Returns A dictionary mapping sample site name (or compartment name) to a tensor whose first dimension corresponds to sample batching.

Return type dict

heuristic (*num_particles=1024*, *ess_threshold=0.5*, *retries=10*)

Finds an initial feasible guess of all latent variables, consistent with observed data. This is needed because not all hypotheses are feasible and HMC needs to start at a feasible solution to progress.

The default implementation attempts to find a feasible state using *SMCFilter* with proprosals from the prior. However this method may be overridden in cases where SMC performs poorly e.g. in high-dimensional models.

Parameters

- **num_particles** (*int*) – Number of particles used for SMC.
- **ess_threshold** (*float*) – Effective sample size threshold for SMC.

Returns A dictionary mapping sample site name to tensor value.

Return type dict

14.2 Example Models

14.2.1 Simple SIR

class SimpleSIRModel (*population*, *recovery_time*, *data*)

Susceptible-Infected-Recovered model.

To customize this model we recommend forking and editing this class.

This is a stochastic discrete-time discrete-state model with three compartments: "S" for susceptible, "I" for infected, and "R" for recovered individuals (the recovered individuals are implicit: `R = population - S - I`) with transitions `S -> I -> R`.

Parameters

- **population** (*int*) – Total `population = S + I + R`.
- **recovery_time** (*float*) – Mean recovery time (duration in state `I`). Must be greater than 1.
- **data** (*iterable*) – Time series of new observed infections. Each time step is Binomial distributed between 0 and the number of `S -> I` transitions. This allows false negative but no false positives.

14.2.2 Simple SEIR

class SimpleSEIRModel(*population*, *incubation_time*, *recovery_time*, *data*)
Susceptible-Exposed-Infected-Recovered model.

To customize this model we recommend forking and editing this class.

This is a stochastic discrete-time discrete-state model with four compartments: "S" for susceptible, "E" for exposed, "I" for infected, and "R" for recovered individuals (the recovered individuals are implicit: `R = population - S - E - I`) with transitions `S -> E -> I -> R`.

Parameters

- **population** (*int*) – Total `population = S + E + I + R`.
- **incubation_time** (*float*) – Mean incubation time (duration in state `E`). Must be greater than 1.
- **recovery_time** (*float*) – Mean recovery time (duration in state `I`). Must be greater than 1.
- **data** (*iterable*) – Time series of new observed infections. Each time step is Binomial distributed between 0 and the number of `S -> E` transitions. This allows false negative but no false positives.

14.2.3 Simple SEIRD

class SimpleSEIRDModel(*population*, *incubation_time*, *recovery_time*, *mortality_rate*, *data*)
Susceptible-Exposed-Infected-Recovered-Dead model.

To customize this model we recommend forking and editing this class.

This is a stochastic discrete-time discrete-state model with four compartments: "S" for susceptible, "E" for exposed, "I" for infected, "D" for deceased individuals, and "R" for recovered individuals (the recovered individuals are implicit: `R = population - S - E - I - D`) with transitions `S -> E -> I -> R` and `I -> D`.

Because the transitions are not simple linear succession, this model implements a custom `compute_flows()` method.

Parameters

- **population** (*int*) – Total `population = S + E + I + R + D`.
- **incubation_time** (*float*) – Mean incubation time (duration in state `E`). Must be greater than 1.
- **recovery_time** (*float*) – Mean recovery time (duration in state `I`). Must be greater than 1.
- **mortality_rate** (*float*) – Portion of infections resulting in death. Must be in the open interval `(0, 1)`.
- **data** (*iterable*) – Time series of new observed infections. Each time step is Binomial distributed between 0 and the number of `S -> E` transitions. This allows false negative but no false positives.

14.2.4 Overdispersed SIR

class OverdispersedSIRModel(*population*, *recovery_time*, *data*)
Generalizes *SimpleSIRModel* with overdispersed distributions.

To customize this model we recommend forking and editing this class.

This adds a single global overdispersion parameter controlling overdispersion of the transition and observation distributions. See *binomial_dist()* and *beta_binomial_dist()* for distributional details. For prior work incorporating overdispersed distributions see [1,2,3,4].

References:

[1] D. Champredon, M. Li, B. Bolker. J. Dushoff (2018) "Two approaches to forecast Ebola synthetic epidemics" https://www.sciencedirect.com/science/article/pii/S1755436517300233

[2] Carrie Reed et al. (2015) "Estimating Influenza Disease Burden from Population-Based Surveillance Data in the United States" https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4349859/

[3] A. Leonard, D. Weissman, B. Greenbaum, E. Ghedin, K. Koelle (2017) "Transmission Bottleneck Size Estimation from Pathogen Deep-Sequencing Data, with an Application to Human Influenza A Virus" https://jvi.asm.org/content/jvi/91/14/e00171-17.full.pdf

[4] A. Miller, N. Foti, J. Lewnard, N. Jewell, C. Guestrin, E. Fox (2020) "Mobility trends provide a leading indicator of changes in SARS-CoV-2 transmission" https://www.medrxiv.org/content/medrxiv/early/2020/05/11/2020.05.07.20094441.full.pdf

Parameters

- **population** (*int*) – Total `population = S + I + R`.
- **recovery_time** (*float*) – Mean recovery time (duration in state `I`). Must be greater than 1.
- **data** (*iterable*) – Time series of new observed infections. Each time step is Binomial distributed between 0 and the number of `S -> I` transitions. This allows false negative but no false positives.

14.2.5 Overdispersed SEIR

class OverdispersedSEIRModel(*population*, *incubation_time*, *recovery_time*, *data*)
Generalizes *SimpleSEIRModel* with overdispersed distributions.

To customize this model we recommend forking and editing this class.

This adds a single global overdispersion parameter controlling overdispersion of the transition and observation distributions. See *binomial_dist()* and *beta_binomial_dist()* for distributional details. For prior work incorporating overdispersed distributions see [1,2,3,4].

References:

[1] D. Champredon, M. Li, B. Bolker. J. Dushoff (2018) "Two approaches to forecast Ebola synthetic epidemics" https://www.sciencedirect.com/science/article/pii/S1755436517300233

[2] Carrie Reed et al. (2015) "Estimating Influenza Disease Burden from Population-Based Surveillance Data in the United States" https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4349859/

[3] A. Leonard, D. Weissman, B. Greenbaum, E. Ghedin, K. Koelle (2017) "Transmission Bottleneck Size Estimation from Pathogen Deep-Sequencing Data, with an Application to Human Influenza A Virus" https://jvi.asm.org/content/jvi/91/14/e00171-17.full.pdf

[4] A. Miller, N. Foti, J. Lewnard, N. Jewell, C. Guestrin, E. Fox (2020) "Mobility trends provide a leading indicator of changes in SARS-CoV-2 transmission" https://www.medrxiv.org/content/medrxiv/early/2020/05/11/2020.05.07.20094441.full.pdf

Parameters

- **population** (*int*) – Total `population = S + E + I + R`.
- **incubation_time** (*float*) – Mean incubation time (duration in state `E`). Must be greater than 1.
- **recovery_time** (*float*) – Mean recovery time (duration in state `I`). Must be greater than 1.
- **data** (*iterable*) – Time series of new observed infections. Each time step is Binomial distributed between 0 and the number of `S -> E` transitions. This allows false negative but no false positives.

14.2.6 Superspreading SIR

class SuperspreadingSIRModel(*population*, *recovery_time*, *data*)

Generalizes *SimpleSIRModel* by adding superspreading effects.

To customize this model we recommend forking and editing this class.

This model accounts for superspreading (overdispersed individual reproductive number) by assuming each infected individual infects BetaBinomial-many susceptible individuals, where the BetaBinomial distribution acts as an overdispersed Binomial distribution, adapting the more standard NegativeBinomial distribution that acts as an overdispersed Poisson distribution [1,2] to the setting of finite populations. To preserve Markov structure, we follow [2] and assume all infections by a single individual occur on the single time step where that individual makes an `I -> R` transition. That is, whereas the *SimpleSIRModel* assumes infected individuals infect *Binomial(S,R/tau)*-many susceptible individuals during each infected time step (over *tau*-many steps on average), this model assumes they infect *BetaBinomial(k,...,S)*-many susceptible individuals but only on the final time step before recovering.

References

[1] J. O. Lloyd-Smith, S. J. Schreiber, P. E. Kopp, W. M. Getz (2005) "Superspreading and the effect of individual variation on disease emergence" https://www.nature.com/articles/nature04153.pdf

[2] Lucy M. Li, Nicholas C. Grassly, Christophe Fraser (2017) "Quantifying Transmission Heterogeneity Using Both Pathogen Phylogenies and Incidence Time Series" https://academic.oup.com/mbe/article/34/11/2982/3952784

Parameters

- **population** (*int*) – Total `population = S + I + R`.
- **recovery_time** (*float*) – Mean recovery time (duration in state `I`). Must be greater than 1.
- **data** (*iterable*) – Time series of new observed infections. Each time step is Binomial distributed between 0 and the number of `S -> I` transitions. This allows false negative but no false positives.

14.2.7 Superspreading SEIR

class SuperspreadingSEIRModel(*population*, *incubation_time*, *recovery_time*, *data*, *, *leaf_times=None*, *coal_times=None*)

Generalizes *SimpleSEIRModel* by adding superspreading effects.

To customize this model we recommend forking and editing this class.

This model accounts for superspreading (overdispersed individual reproductive number) by assuming each infected individual infects BetaBinomial-many susceptible individuals, where the BetaBinomial distribution acts as an overdispersed Binomial distribution, adapting the more standard NegativeBinomial distribution that acts as an overdispersed Poisson distribution [1,2] to the setting of finite populations. To preserve Markov structure, we follow [2] and assume all infections by a single individual occur on the single time step where that individual makes an `I -> R` transition. That is, whereas the *SimpleSEIRModel* assumes infected individuals infect *Binomial(S,R/tau)*-many susceptible individuals during each infected time step (over *tau*-many steps on average), this model assumes they infect *BetaBinomial(k,...,S)*-many susceptible individuals but only on the final time step before recovering.

This model also adds an optional likelihood for observed phylogenetic data in the form of coalescent times. These are provided as a pair `(leaf_times, coal_times)` of times at which genomes are sequenced and lineages coalesce, respectively. We incorporate this data using the *CoalescentRateLikelihood* with base coalescence rate computed from the `S` and `I` populations. This likelihood is independent across time and preserves the Markov propert needed for inference.

References

[1] J. O. Lloyd-Smith, S. J. Schreiber, P. E. Kopp, W. M. Getz (2005) "Superspreading and the effect of individual variation on disease emergence" https://www.nature.com/articles/nature04153.pdf

[2] Lucy M. Li, Nicholas C. Grassly, Christophe Fraser (2017) "Quantifying Transmission Heterogeneity Using Both Pathogen Phylogenies and Incidence Time Series" https://academic.oup.com/mbe/article/34/11/2982/3952784

Parameters

- **population** (*int*) – Total `population = S + E + I + R`.
- **incubation_time** (*float*) – Mean incubation time (duration in state `E`). Must be greater than 1.
- **recovery_time** (*float*) – Mean recovery time (duration in state `I`). Must be greater than 1.
- **data** (*iterable*) – Time series of new observed infections. Each time step is Binomial distributed between 0 and the number of `S -> E` transitions. This allows false negative but no false positives.

14.2.8 Heterogeneous SIR

class HeterogeneousSIRModel(*population*, *recovery_time*, *data*)

Generalizes *SimpleSIRModel* by allowing `Rt` and `rho` to vary in time.

To customize this model we recommend forking and editing this class.

In this model, the response rate `rho` is piecewise constant with unknown value over three pieces. The reproductive number `Rt` is a product of a constant `R0` with a factor `beta` that drifts via Brownian motion in log space. Both `rho` and `Rt` are available as time series.

Parameters

- **population** (*int*) – Total `population = S + I + R`.
- **recovery_time** (*float*) – Mean recovery time (duration in state `I`). Must be greater than 1.
- **data** (*iterable*) – Time series of new observed infections. Each time step is Binomial distributed between 0 and the number of `S -> I` transitions. This allows false negative but no false positives.

14.2.9 Sparse SIR

class SparseSIRModel(*population*, *recovery_time*, *data*, *mask*)

Generalizes *SimpleSIRModel* to allow sparsely observed infections.

To customize this model we recommend forking and editing this class.

This model allows observations of **cumulative** infections at uneven time intervals. To preserve Markov structure (and hence tractable inference) this model adds an auxiliary compartment `O` denoting the fully-observed cumulative number of observations at each time point. At observed times (when `mask[t] == True`) `O` must exactly match the provided data; between observed times `O` stochastically imputes the provided data.

This model demonstrates how to implement a custom `compute_flows()` method. A custom method is needed in this model because inhabitants of the `S` compartment can transition to both the `I` and `O` compartments, allowing duplication.

Parameters

- **population** (*int*) – Total `population = S + I + R`.
- **recovery_time** (*float*) – Mean recovery time (duration in state `I`). Must be greater than 1.
- **data** (*iterable*) – Time series of **cumulative** observed infections. Whenever `mask[t] == True`, `data[t]` corresponds to an observation; otherwise `data[t]` can be arbitrary, e.g. NAN.
- **mask** (*iterable*) – Boolean time series denoting whether an observation is made at each time step. Should satisfy `len(mask) == len(data)`.

14.2.10 Unknown Start SIR

class UnknownStartSIRModel(*population*, *recovery_time*, *pre_obs_window*, *data*)

Generalizes *SimpleSIRModel* by allowing unknown date of first infection.

To customize this model we recommend forking and editing this class.

This model demonstrates:

1. How to incorporate spontaneous infections from external sources;
2. How to incorporate time-varying piecewise `rho` by supporting forecasting in `transition()`.
3. How to override the `predict()` method to compute extra statistics.

Parameters

- **population** (*int*) – Total `population = S + I + R`.
- **recovery_time** (*float*) – Mean recovery time (duration in state `I`). Must be greater than 1.

- **pre_obs_window** (*int*) – Number of time steps before beginning `data` where the initial infection may have occurred. Must be positive.
- **data** (*iterable*) – Time series of new observed infections. Each time step is Binomial distributed between 0 and the number of `S -> I` transitions. This allows false negative but no false positives.

14.2.11 Regional SIR

class RegionalSIRModel(*population*, *coupling*, *recovery_time*, *data*)

Generalizes *SimpleSIRModel* to simultaneously model multiple regions with weak coupling across regions.

To customize this model we recommend forking and editing this class.

Regions are coupled by a `coupling` matrix with entries in `[0,1]`. The all ones matrix is equivalent to a single region. The identity matrix is equivalent to a set of independent regions. This need not be symmetric, but symmetric matrices are probably more physically plausible. The expected number of new infections each time step `S2I` is Binomial distributed with mean:

```
E[S2I] = S (1 - (1 - R0 / (population @ coupling)) ** (I @ coupling))
       ≈ R0 S (I @ coupling) / (population @ coupling)  # for small I
```

Thus in a nearly entirely susceptible population, a single infected individual infects approximately `R0` new individuals on average, independent of `coupling`.

This model demonstrates:

1. How to create a regional model with a `population` vector.
2. How to model both homogeneous parameters (here `R0`) and heterogeneous parameters with hierarchical structure (here `rho`) using `self.region_plate`.
3. How to approximately couple regions in `transition()` using `state["I_approx"]`.

Parameters

- **population** (*torch.Tensor*) – Tensor of per-region populations, defining `population = S + I + R`.
- **coupling** (*torch.Tensor*) – Pairwise coupling matrix. Entries should be in `[0,1]`.
- **recovery_time** (*float*) – Mean recovery time (duration in state `I`). Must be greater than 1.
- **data** (*iterable*) – Time x Region sized tensor of new observed infections. Each time step is vector of Binomials distributed between 0 and the number of `S -> I` transitions. This allows false negative but no false positives.

14.2.12 Heterogeneous Regional SIR

class HeterogeneousRegionalSIRModel(*population*, *coupling*, *recovery_time*, *data*)

Generalizes *RegionalSIRModel* by allowing `Rt` and `rho` to vary in time.

To customize this model we recommend forking and editing this class.

In this model, the response rate `rho` varies across time and region, whereas the reproductive number `Rt` varies in time but is shared among regions. Both parameters drift according to transformed Brownian motion with learned drift rate.

This model demonstrates how to model hierarchical latent time series, other than compartmental variables.

Parameters

- **population** (*torch.Tensor*) – Tensor of per-region populations, defining `population = S + I + R`.
- **coupling** (*torch.Tensor*) – Pairwise coupling matrix. Entries should be in `[0,1]`.
- **recovery_time** (*float*) – Mean recovery time (duration in state `I`). Must be greater than 1.
- **data** (*iterable*) – Time x Region sized tensor of new observed infections. Each time step is vector of Binomials distributed between 0 and the number of `S -> I` transitions. This allows false negative but no false positives.

14.3 Distributions

set_approx_sample_thresh(*thresh*)

EXPERIMENTAL Context manager / decorator to temporarily set the global default value of `Binomial.approx_sample_thresh`, thereby decreasing the computational complexity of sampling from *Binomial*, *BetaBinomial*, *ExtendedBinomial*, *ExtendedBetaBinomial*, and distributions returned by *infection_dist()*.

This is useful for sampling from very large `total_count`.

This is used internally by *CompartmentalModel*.

Parameters **thresh** (*int or float.*) – New temporary threshold.

set_approx_log_prob_tol(*tol*)

EXPERIMENTAL Context manager / decorator to temporarily set the global default value of `Binomial.approx_log_prob_tol` and `BetaBinomial.approx_log_prob_tol`, thereby decreasing the computational complexity of scoring *Binomial* and *BetaBinomial* distributions.

This is used internally by *CompartmentalModel*.

Parameters **tol** (*int or float.*) – New temporary tolold.

binomial_dist(*total_count*, *probs*, *, *overdispersion=0.0*)

Returns a Beta-Binomial distribution that is an overdispersed version of a Binomial distribution, according to a parameter `overdispersion`, typically set in the range 0.1 to 0.5.

This is useful for (1) fitting real data that is overdispersed relative to a Binomial distribution, and (2) relaxing models of large populations to improve inference. In particular the `overdispersion` parameter lower bounds the relative uncertainty in stochastic models such that increasing population leads to a limiting scale-free dynamical system with bounded stochasticity, in contrast to Binomial-based SDEs that converge to deterministic ODEs in the large population limit.

This parameterization satisfies the following properties:

1. Variance increases monotonically in `overdispersion`.
2. `overdispersion = 0` results in a Binomial distribution.
3. `overdispersion` lower bounds the relative uncertainty `std_dev / (total_count * p * q)`, where `probs = p = 1 - q`, and serves as an asymptote for relative uncertainty as `total_count` $\to \infty$. This contrasts the Binomial whose relative uncertainty tends to zero.
4. If `X ~ binomial_dist(n, p, overdispersion=`σ`)` then in the large population limit `n` $\to \infty$, the scaled random variable `X / n` converges in distribution to `LogitNormal(log(p/(1-p)),` σ`)`.

To achieve these properties we set `p = probs`, `q = 1 - p`, and:

```
concentration = 1 / (p * q * overdispersion**2) - 1
```

Parameters

- **total_count** (*int or torch.Tensor*) – Number of Bernoulli trials.
- **probs** (*float or torch.Tensor*) – Event probabilities.
- **overdispersion** (*float or torch.tensor*) – Amount of overdispersion, in the half open interval [0,2). Defaults to zero.

beta_binomial_dist(*concentration1*, *concentration0*, *total_count*, ***, *overdispersion=0.0*)

Returns a Beta-Binomial distribution that is an overdispersed version of a the usual Beta-Binomial distribution, according to an extra parameter `overdispersion`, typically set in the range 0.1 to 0.5.

Parameters

- **concentration1** (*float or torch.Tensor*) – 1st concentration parameter (alpha) for the Beta distribution.
- **concentration0** (*float or torch.Tensor*) – 2nd concentration parameter (beta) for the Beta distribution.
- **total_count** (*float or torch.Tensor*) – Number of Bernoulli trials.
- **overdispersion** (*float or torch.tensor*) – Amount of overdispersion, in the half open interval [0,2). Defaults to zero.

infection_dist(***, *individual_rate*, *num_infectious*, *num_susceptible=inf*, *population=inf*, *concentration=inf*, *overdispersion=0.0*)

Create a *Distribution* over the number of new infections at a discrete time step.

This returns a Poisson, Negative-Binomial, Binomial, or Beta-Binomial distribution depending on whether `population` and `concentration` are finite. In Pyro models, the population is usually finite. In the limit `population` $\to \infty$ and `num_susceptible/population` $\to 1$, the Binomial converges to Poisson and the Beta-Binomial converges to Negative-Binomial. In the limit `concentration` $\to \infty$, the Negative-Binomial converges to Poisson and the Beta-Binomial converges to Binomial.

The overdispersed distributions (Negative-Binomial and Beta-Binomial returned when `concentration` $< \infty$) are useful for modeling superspreader individuals [1,2]. The finitely supported distributions Binomial and Negative-Binomial are useful in small populations and in probabilistic programming systems where truncation or censoring are expensive [3].

References

[1] J. O. Lloyd-Smith, S. J. Schreiber, P. E. Kopp, W. M. Getz (2005) "Superspreading and the effect of individual variation on disease emergence" https://www.nature.com/articles/nature04153.pdf

[2] Lucy M. Li, Nicholas C. Grassly, Christophe Fraser (2017) "Quantifying Transmission Heterogeneity Using Both Pathogen Phylogenies and Incidence Time Series" https://academic.oup.com/mbe/article/34/11/2982/3952784

[3] Lawrence Murray et al. (2018) "Delayed Sampling and Automatic Rao-Blackwellization of Probabilistic Programs" https://arxiv.org/pdf/1708.07787.pdf

Parameters

- **individual_rate** – The mean number of infections per infectious individual per time step in the limit of large population, equal to `R0 / tau` where `R0` is the basic reproductive number and `tau` is the mean duration of infectiousness.

- **num_infectious** – The number of infectious individuals at this time step, sometimes `I`, sometimes `E+I`.
- **num_susceptible** – The number `S` of susceptible individuals at this time step. This defaults to an infinite population.
- **population** – The total number of individuals in a population. This defaults to an infinite population.
- **concentration** – The concentration or dispersion parameter `k` in overdispersed models of superspreaders [1,2]. This defaults to minimum variance `concentration = ∞`.
- **overdispersion** (*float or torch.tensor*) – Amount of overdispersion, in the half open interval [0,2). Defaults to zero.

class CoalescentRateLikelihood(*leaf_times*, *coal_times*, *duration*, *, *validate_args=None*)

Bases: `object`

EXPERIMENTAL This is not a *Distribution*, but acts as a transposed version of *CoalescentTimesWithRate* making the elements of `rate_grid` independent and thus compatible with `plate` and `poutine.markov`. For non-batched inputs the following are all equivalent likelihoods:

```
# Version 1.
pyro.sample("coalescent",
            CoalescentTimesWithRate(leaf_times, rate_grid),
            obs=coal_times)

# Version 2. using pyro.plate
likelihood = CoalescentRateLikelihood(leaf_times, coal_times, len(rate_grid))
with pyro.plate("time", len(rate_grid)):
    pyro.factor("coalescent", likelihood(rate_grid))

# Version 3. using pyro.markov
likelihood = CoalescentRateLikelihood(leaf_times, coal_times, len(rate_grid))
for t in pyro.markov(range(len(rate_grid))):
    pyro.factor("coalescent_{}".format(t), likelihood(rate_grid[t], t))
```

The third version is useful for e.g. *SMCFilter* where `rate_grid` might be computed sequentially.

Parameters

- **leaf_times** (*torch.Tensor*) – Tensor of times of sampling events, i.e. leaf nodes in the phylogeny. These can be arbitrary real numbers with arbitrary order and duplicates.
- **coal_times** (*torch.Tensor*) – A tensor of coalescent times. These denote sets of size `leaf_times.size(-1) - 1` along the trailing dimension and should be sorted along that dimension.
- **duration** (*int*) – Size of the rate grid, `rate_grid.size(-1)`.

__call__(*rate_grid*, *t=slice(None, None, None)*)

Computes the likelihood of [1] equations 7-9 for one or all time points.

References

[1] A. Popinga, T. Vaughan, T. Statler, A.J. Drummond (2014) "Inferring epidemiological dynamics with Bayesian coalescent inference: The merits of deterministic and stochastic models" https://arxiv.org/pdf/1407.1792.pdf

Parameters

- **rate_grid** (*torch.Tensor*) – Tensor of base coalescent rates (pairwise rate of coalescence). For example in a simple SIR model this might be `beta S / I`. The rightmost dimension is time, and this tensor represents a (batch of) rates that are piecwise constant in time.
- **time** (*int or slice*) – Optional time index by which the input was sliced, as in `rate_grid[..., t]` This can be an integer for sequential models or `slice(None)` for vectorized models.

Returns Likelihood `p(coal_times | leaf_times, rate_grid)`, or a part of that likelihood corresponding to a single time step.

Return type torch.Tensor

bio_phylo_to_times(*tree*, *, *get_time=None*)

Extracts coalescent summary statistics from a phylogeny, suitable for use with *CoalescentRateLikelihood*.

Parameters

- **tree** (*Bio.Phylo.BaseTree.Clade*) – A phylogenetic tree.
- **get_time** (*callable*) – Optional function to extract the time point of each sub-`Clade`. If absent, times will be computed by cumulative *.branch_length*.

Returns A pair of `Tensor` s `(leaf_times, coal_times)` where `leaf_times` are times of sampling events (leaf nodes in the phylogenetic tree) and `coal_times` are times of coalescences (leaf nodes in the phylogenetic binary tree).

Return type tuple

CHAPTER 15

Pyro Examples

15.1 Datasets

15.1.1 Multi MNIST

This script generates a dataset similar to the Multi-MNIST dataset described in [1].

[1] Eslami, SM Ali, et al. "Attend, infer, repeat: Fast scene understanding with generative models." Advances in Neural Information Processing Systems. 2016.

imresize(*arr*, *size*)

sample_one(*canvas_size*, *mnist*)

sample_multi(*num_digits*, *canvas_size*, *mnist*)

mk_dataset(*n*, *mnist*, *max_digits*, *canvas_size*)

load_mnist(*root_path*)

load(*root_path*)

15.1.2 BART Ridership

load_bart_od()

Load a dataset of hourly origin-destination ridership counts for every pair of BART stations during the years 2011-2019.

Source https://www.bart.gov/about/reports/ridership

This downloads the dataset the first time it is called. On subsequent calls this reads from a local cached file `.pkl.bz2`. This attempts to download a preprocessed compressed cached file maintained by the Pyro team. On cache hit this should be very fast. On cache miss this falls back to downloading the original data source and preprocessing the dataset, requiring about 350MB of file transfer, storing a few GB of temp files, and taking upwards of 30 minutes.

Returns

a dataset is a dictionary with fields:

- ”stations”: a list of strings of station names
- ”start_date”: a `datetime.datetime` for the first observaion
- ”counts”: a `torch.FloatTensor` of ridership counts, with shape `(num_hours, len(stations), len(stations))`.

load_fake_od()
Create a tiny synthetic dataset for smoke testing.

15.2 Utilities

get_data_loader(*dataset_name*, *data_dir*, *batch_size=1*, *dataset_transforms=None*, *is_training_set=True*, *shuffle=True*)

print_and_log(*logger*, *msg*)

get_data_directory(*filepath=None*)

CHAPTER 16

Forecasting

`pyro.contrib.forecast` is a lightweight framework for experimenting with a restricted class of time series models and inference algorithms using familiar Pyro modeling syntax and PyTorch neural networks.

Models include hierarchical multivariate heavy-tailed time series of ~1000 time steps and ~1000 separate series. Inference combines subsample-compatible variational inference with Gaussian variable elimination based on the *GaussianHMM* class. Inference using Hamiltonian Monte Carlo sampling is also supported with *HMCForecaster*. Forecasts are in the form of joint posterior samples at multiple future time steps.

Hierarchical models use the familiar `plate` syntax for general hierarchical modeling in Pyro. Plates can be subsampled, enabling training of joint models over thousands of time series. Multivariate observations are handled via multivariate likelihoods like *MultivariateNormal*, *GaussianHMM*, or *LinearHMM*. Heavy tailed models are possible by using *StudentT* or *Stable* likelihoods, possibly together with *LinearHMM* and reparameterizers including *StudentTReparam*, *StableReparam*, and *LinearHMMReparam*.

Seasonality can be handled using the helpers *periodic_repeat()*, *periodic_cumsum()*, and *periodic_features()*.

See *pyro.contrib.timeseries* for ways to construct temporal Gaussian processes useful as likelihoods.

For example usage see:

- The univariate forecasting tutorial
- The state space modeling tutorial
- The hierarchical forecasting tutorial
- The forecasting example

16.1 Forecaster Interface

class ForecastingModel

Bases: *pyro.nn.module.PyroModule*

Abstract base class for forecasting models.

Derived classes must implement the *model()* method.

model(*zero_data*, *covariates*)
Generative model definition.

Implementations must call the *predict()* method exactly once.

Implementations must draw all time-dependent noise inside the *time_plate()*. The prediction passed to *predict()* must be a deterministic function of noise tensors that are independent over time. This requirement is slightly more general than state space models.

Parameters

- **zero_data** (*Tensor*) – A zero tensor like the input data, but extended to the duration of the *time_plate()*. This allows models to depend on the shape and device of data but not its value.
- **covariates** (*Tensor*) – A tensor of covariates with time dimension -2.

Returns Return value is ignored.

time_plate

Returns A plate named "time" with size `covariates.size(-2)` and `dim=-1`. This is available only during model execution.

Return type `plate`

predict(*noise_dist*, *prediction*)
Prediction function, to be called by *model()* implementations.

This should be called outside of the *time_plate()*.

This is similar to an observe statement in Pyro:

```
pyro.sample("residual", noise_dist,
            obs=(data - prediction))
```

but with (1) additional reshaping logic to allow time-dependent `noise_dist` (most often a *GaussianHMM* or variant); and (2) additional logic to allow only a partial observation and forecast the remaining data.

Parameters

- **noise_dist** (`Distribution`) – A noise distribution with `.event_dim in {0, 1, 2}`. `noise_dist` is typically zero-mean or zero-median or zero-mode or somehow centered.
- **prediction** (*Tensor*) – A prediction for the data. This should have the same shape as `data`, but broadcastable to full duration of the `covariates`.

class Forecaster(*model*, *data*, *covariates*, ***, *guide=None*, *init_loc_fn=<function init_to_sample>*, *init_scale=0.1*, *create_plates=None*, *optim=None*, *learning_rate=0.01*, *betas=(0.9, 0.99)*, *learning_rate_decay=0.1*, *clip_norm=10.0*, *time_reparam=None*, *dct_gradients=False*, *subsample_aware=False*, *num_steps=1001*, *num_particles=1*, *vectorize_particles=True*, *warm_start=False*, *log_every=100*)
Bases: `torch.nn.modules.module.Module`

Forecaster for a *ForecastingModel* using variational inference.

On initialization, this fits a distribution using variational inference over latent variables and exact inference over the noise distribution, typically a *GaussianHMM* or variant.

After construction this can be called to generate sample forecasts.

Variables **losses** (*list*) – A list of losses recorded during training, typically used to debug convergence. Defined by `loss = -elbo / data.numel()`.

Parameters

- **model** (ForecastingModel) – A forecasting model subclass instance.
- **data** (*Tensor*) – A tensor dataset with time dimension -2.
- **covariates** (*Tensor*) – A tensor of covariates with time dimension -2. For models not using covariates, pass a shaped empty tensor `torch.empty(duration, 0)`.
- **guide** (PyroModule) – Optional guide instance. Defaults to a *AutoNormal*.
- **init_loc_fn** (*callable*) – A per-site initialization function for the *AutoNormal* guide. Defaults to *init_to_sample()*. See *Initialization* section for available functions.
- **init_scale** (*float*) – Initial uncertainty scale of the *AutoNormal* guide.
- **create_plates** (*callable*) – An optional function to create plates for subsampling with the *AutoNormal* guide.
- **optim** (PyroOptim) – An optional Pyro optimizer. Defaults to a freshly constructed *DCTAdam*.
- **learning_rate** (*float*) – Learning rate used by *DCTAdam*.
- **betas** (*tuple*) – Coefficients for running averages used by *DCTAdam*.
- **learning_rate_decay** (*float*) – Learning rate decay used by *DCTAdam*. Note this is the total decay over all `num_steps`, not the per-step decay factor.
- **clip_norm** (*float*) – Norm used for gradient clipping during optimization. Defaults to 10.0.
- **time_reparam** (*str*) – If not None (default), reparameterize all time-dependent variables via the Haar wavelet transform (if "haar") or the discrete cosine transform (if "dct").
- **dct_gradients** (*bool*) – Whether to discrete cosine transform gradients in *DCTAdam*. Defaults to False.
- **subsample_aware** (*bool*) – whether to update gradient statistics only for those elements that appear in a subsample. This is used by *DCTAdam*.
- **num_steps** (*int*) – Number of *SVI* steps.
- **num_particles** (*int*) – Number of particles used to compute the *ELBO*.
- **vectorize_particles** (*bool*) – If `num_particles > 1`, determines whether to vectorize computation of the *ELBO*. Defaults to True. Set to False for models with dynamic control flow.
- **warm_start** (*bool*) – Whether to warm start parameters from a smaller time window. Note this may introduce statistical leakage; usage is recommended for model exploration purposes only and should be disabled when publishing metrics.
- **log_every** (*int*) – Number of training steps between logging messages.

__call__(*data*, *covariates*, *num_samples*, *batch_size=None*)

Samples forecasted values of data for time steps in `[t1,t2)`, where `t1 = data.size(-2)` is the duration of observed data and `t2 = covariates.size(-2)` is the extended duration of covariates. For example to forecast 7 days forward conditioned on 30 days of observations, set `t1=30` and `t2=37`.

Parameters

- **data** (*Tensor*) – A tensor dataset with time dimension -2.
- **covariates** (*Tensor*) – A tensor of covariates with time dimension -2. For models not using covariates, pass a shaped empty tensor `torch.empty(duration, 0)`.
- **num_samples** (*int*) – The number of samples to generate.
- **batch_size** (*int*) – Optional batch size for sampling. This is useful for generating many samples from models with large memory footprint. Defaults to `num_samples`.

Returns A batch of joint posterior samples of shape `(num_samples,1,...,1) + data.shape[:-2] + (t2-t1,data.size(-1))`, where the `1`'s are inserted to avoid conflict with model plates.

Return type Tensor

class HMCForecaster(*model*, *data*, *covariates=None*, ***, *num_warmup=1000*, *num_samples=1000*, *num_chains=1*, *time_reparam=None*, *dense_mass=False*, *jit_compile=False*, *max_tree_depth=10*)

Bases: `torch.nn.modules.module.Module`

Forecaster for a *ForecastingModel* using Hamiltonian Monte Carlo.

On initialization, this will run `NUTS` sampler to get posterior samples of the model.

After construction, this can be called to generate sample forecasts.

Parameters

- **model** (`ForecastingModel`) – A forecasting model subclass instance.
- **data** (*Tensor*) – A tensor dataset with time dimension -2.
- **covariates** (*Tensor*) – A tensor of covariates with time dimension -2. For models not using covariates, pass a shaped empty tensor `torch.empty(duration, 0)`.
- **num_warmup** (*int*) – number of MCMC warmup steps.
- **num_samples** (*int*) – number of MCMC samples.
- **num_chains** (*int*) – number of parallel MCMC chains.
- **dense_mass** (*bool*) – a flag to control whether the mass matrix is dense or diagonal. Defaults to False.
- **time_reparam** (*str*) – If not None (default), reparameterize all time-dependent variables via the Haar wavelet transform (if "haar") or the discrete cosine transform (if "dct").
- **jit_compile** (*bool*) – whether to use the PyTorch JIT to trace the log density computation, and use this optimized executable trace in the integrator. Defaults to False.
- **max_tree_depth** (*int*) – Max depth of the binary tree created during the doubling scheme of the `NUTS` sampler. Defaults to 10.

__call__(*data*, *covariates*, *num_samples*, *batch_size=None*)

Samples forecasted values of data for time steps in `[t1,t2)`, where `t1 = data.size(-2)` is the duration of observed data and `t2 = covariates.size(-2)` is the extended duration of covariates. For example to forecast 7 days forward conditioned on 30 days of observations, set `t1=30` and `t2=37`.

Parameters

- **data** (*Tensor*) – A tensor dataset with time dimension -2.
- **covariates** (*Tensor*) – A tensor of covariates with time dimension -2. For models not using covariates, pass a shaped empty tensor `torch.empty(duration, 0)`.
- **num_samples** (*int*) – The number of samples to generate.

- **batch_size** (*int*) – Optional batch size for sampling. This is useful for generating many samples from models with large memory footprint. Defaults to `num_samples`.

Returns A batch of joint posterior samples of shape `(num_samples,1,...,1) + data.shape[:-2] + (t2-t1,data.size(-1))`, where the `1`'s are inserted to avoid conflict with model plates.

Return type Tensor

16.2 Evaluation

eval_mae(*pred*, *truth*)
Evaluate mean absolute error, using sample median as point estimate.

Parameters

- **pred** (*torch.Tensor*) – Forecasted samples.
- **truth** (*torch.Tensor*) – Ground truth.

Return type float

eval_rmse(*pred*, *truth*)
Evaluate root mean squared error, using sample mean as point estimate.

Parameters

- **pred** (*torch.Tensor*) – Forecasted samples.
- **truth** (*torch.Tensor*) – Ground truth.

Return type float

eval_crps(*pred*, *truth*)
Evaluate continuous ranked probability score, averaged over all data elements.

References

[1] Tilmann Gneiting, Adrian E. Raftery (2007) *Strictly Proper Scoring Rules, Prediction, and Estimation* https://www.stat.washington.edu/raftery/Research/PDF/Gneiting2007jasa.pdf

Parameters

- **pred** (*torch.Tensor*) – Forecasted samples.
- **truth** (*torch.Tensor*) – Ground truth.

Return type float

backtest(*data*, *covariates*, *model_fn*, **, forecaster_fn=<class 'pyro.contrib.forecast.forecaster.Forecaster'>*, *metrics=None*, *transform=None*, *train_window=None*, *min_train_window=1*, *test_window=None*, *min_test_window=1*, *stride=1*, *seed=1234567890*, *num_samples=100*, *batch_size=None*, *forecaster_options={}*)
Backtest a forecasting model on a moving window of (train,test) data.

Parameters

- **data** (*Tensor*) – A tensor dataset with time dimension -2.
- **covariates** (*Tensor*) – A tensor of covariates with time dimension -2. For models not using covariates, pass a shaped empty tensor `torch.empty(duration, 0)`.
- **model_fn** (*callable*) – Function that returns an *ForecastingModel* object.

- **forecaster_fn** (*callable*) – Function that returns a forecaster object (for example, *Forecaster* or *HMCForecaster*) given arguments model, training data, training covariates and keyword arguments defined in *forecaster_options*.
- **metrics** (*dict*) – A dictionary mapping metric name to metric function. The metric function should input a forecast `pred` and ground `truth` and can output anything, often a number. Example metrics include: *eval_mae()*, *eval_rmse()*, and *eval_crps()*.
- **transform** (*callable*) – An optional transform to apply before computing metrics. If provided this will be applied as `pred, truth = transform(pred, truth)`.
- **train_window** (*int*) – Size of the training window. Be default trains from beginning of data. This must be None if forecaster is *Forecaster* and `forecaster_options["warm_start"]` is true.
- **min_train_window** (*int*) – If `train_window` is None, this specifies the min training window size. Defaults to 1.
- **test_window** (*int*) – Size of the test window. By default forecasts to end of data.
- **min_test_window** (*int*) – If `test_window` is None, this specifies the min test window size. Defaults to 1.
- **stride** (*int*) – Optional stride for test/train split. Defaults to 1.
- **seed** (*int*) – Random number seed.
- **num_samples** (*int*) – Number of samples for forecast. Defaults to 100.
- **batch_size** (*int*) – Batch size for forecast sampling. Defaults to `num_samples`.
- **forecaster_options** (*dict or callable*) – Options dict to pass to forecaster, or callable inputting time window `t0,t1,t2` and returning such a dict. See `Forecaster` for details.

Returns A list of dictionaries of evaluation data. Caller is responsible for aggregating the per-window metrics. Dictionary keys include: train begin time “t0”, train/test split time “t1”, test end time “t2”, “seed”, “num_samples”, “train_walltime”, “test_walltime”, and one key for each metric.

Return type list

CHAPTER 17

Funsor-based Pyro

plate (**args*, ***kwargs*)

17.1 Effect handlers

enum (*fn=None*, **args*, ***kwargs*)
Convenient wrapper of *EnumMessenger*

This version of EnumMessenger uses to_data to allocate a fresh enumeration dim for each discrete sample site.

markov (*fn=None*, **args*, ***kwargs*)
Convenient wrapper of *MarkovMessenger*

Handler for converting to/from funsors consistent with Pyro's positional batch dimensions.

Parameters

- **history** (*int*) – The number of previous contexts visible from the current context. Defaults to 1. If zero, this is similar to `pyro.plate`.
- **keep** (*bool*) – If true, frames are replayable. This is important when branching: if `keep=True`, neighboring branches at the same level can depend on each other; if `keep=False`, neighboring branches are independent (conditioned on their shared ancestors).

named (*fn=None*, **args*, ***kwargs*)
Convenient wrapper of `NamedMessenger`

Base effect handler class for the :func:~'pyro.contrib.funsor.to_funsor' and :func:~'pyro.contrib.funsor.to_data' primitives. Any effect handlers that invoke these primitives internally or wrap code that does should inherit from `NamedMessenger`.

This design ensures that the global name-dim mapping is reset upon handler exit rather than potentially persisting until the entire program terminates.

plate (*fn=None*, **args*, ***kwargs*)
Convenient wrapper of *PlateMessenger*

Combines new IndepMessenger implementation with existing BroadcastMessenger. Should eventually be a drop-in replacement for pyro.plate.

replay (*fn=None*, **args*, ***kwargs*)
Convenient wrapper of *ReplayMessenger*

This version of ReplayMessenger is almost identical to the original version, except that it calls to_data on the replayed funsor values. This may result in different unpacked shapes, but should produce correct allocations.

trace (*fn=None*, **args*, ***kwargs*)
Convenient wrapper of *TraceMessenger*

Setting `pack_online=True` packs online instead of after the fact, converting all distributions and values to Funsors as soon as they are available.

Setting `pack_online=False` computes information necessary to do packing after execution. Each sample site is annotated with a "dim_to_name" dictionary, which can be passed directly to funsor.to_funsor.

class NamedMessenger (*first_available_dim=None*)
Bases: *pyro.poutine.reentrant_messenger.ReentrantMessenger*

Base effect handler class for the :func:~'pyro.contrib.funsor.to_funsor' and :func:~'pyro.contrib.funsor.to_data' primitives. Any effect handlers that invoke these primitives internally or wrap code that does should inherit from `NamedMessenger`.

This design ensures that the global name-dim mapping is reset upon handler exit rather than potentially persisting until the entire program terminates.

class MarkovMessenger (*history=1*, *keep=False*)
Bases: *pyro.contrib.funsor.handlers.named_messenger.NamedMessenger*

Handler for converting to/from funsors consistent with Pyro's positional batch dimensions.

Parameters

- **history** (*int*) – The number of previous contexts visible from the current context. Defaults to 1. If zero, this is similar to `pyro.plate`.
- **keep** (*bool*) – If true, frames are replayable. This is important when branching: if `keep=True`, neighboring branches at the same level can depend on each other; if `keep=False`, neighboring branches are independent (conditioned on their shared ancestors).

class GlobalNamedMessenger (*first_available_dim=None*)
Bases: *pyro.contrib.funsor.handlers.named_messenger.NamedMessenger*

Base class for any new effect handlers that use the :func:~'pyro.contrib.funsor.to_funsor' and :func:~'pyro.contrib.funsor.to_data' primitives to allocate *DimType.GLOBAL* or *DimType.VISIBLE* dimensions.

Serves as a manual "scope" for dimensions that should not be recycled by :class:~'MarkovMessenger': global dimensions will be considered active until the innermost `GlobalNamedMessenger` under which they were initially allocated exits.

to_funsor (*x*, *output=None*, *dim_to_name=None*, *dim_type=<DimType.LOCAL: 0>*)

to_data (*x*, *name_to_dim=None*, *dim_type=<DimType.LOCAL: 0>*)

class StackFrame (*name_to_dim*, *dim_to_name*, *history=1*, *keep=False*)
Bases: `object`

Consistent bidirectional mapping between integer positional dimensions and names. Can be queried like a dictionary (value = frame[key], frame[key] = value).

class DimType
Bases: enum.Enum

Enumerates the possible types of dimensions to allocate

LOCAL = 0

GLOBAL = 1

VISIBLE = 2

class DimRequest(*value*, *dim_type*)
Bases: tuple

dim_type
Alias for field number 1

value
Alias for field number 0

class DimStack
Bases: object

Single piece of global state to keep track of the mapping between names and dimensions.

Replaces the plate DimAllocator, the enum EnumAllocator, the stack in MarkovMessenger, _param_dims and _value_dims in EnumMessenger, and dim_to_symbol in msg['infer']

MAX_DIM = -25

DEFAULT_FIRST_DIM = -5

set_first_available_dim(*dim*)

push_global(*frame*)

pop_global()

push_iter(*frame*)

pop_iter()

push_local(*frame*)

pop_local()

global_frame

local_frame

current_write_env

current_read_env
Collect all frames necessary to compute the full name <–> dim mapping and interpret Funsor inputs or batch shapes at any point in a computation.

allocate(*key_to_value_request*)

names_from_batch_shape(*batch_shape*, *dim_type=<DimType.LOCAL: 0>*)

CHAPTER 18

Gaussian Processes

See the Gaussian Processes tutorial for an introduction.

class Parameterized

Bases: *pyro.nn.module.PyroModule*

A wrapper of *PyroModule* whose parameters can be set constraints, set priors.

By default, when we set a prior to a parameter, an auto Delta guide will be created. We can use the method *autoguide()* to setup other auto guides.

Example:

```
>>> class Linear(Parameterized):
...     def __init__(self, a, b):
...         super().__init__()
...         self.a = Parameter(a)
...         self.b = Parameter(b)
...
...     def forward(self, x):
...         return self.a * x + self.b
...
>>> linear = Linear(torch.tensor(1.), torch.tensor(0.))
>>> linear.a = PyroParam(torch.tensor(1.), constraints.positive)
>>> linear.b = PyroSample(dist.Normal(0, 1))
>>> linear.autoguide("b", dist.Normal)
>>> assert "a_unconstrained" in dict(linear.named_parameters())
>>> assert "b_loc" in dict(linear.named_parameters())
>>> assert "b_scale_unconstrained" in dict(linear.named_parameters())
```

Note that by default, data of a parameter is a float `torch.Tensor` (unless we use `torch.set_default_tensor_type()` to change default tensor type). To cast these parameters to a correct data type or GPU device, we can call methods such as `double()` or `cuda()`. See `torch.nn.Module` for more information.

set_prior(*name*, *prior*)

Sets prior for a parameter.

Parameters

- **name** (*str*) – Name of the parameter.
- **prior** (*Distribution*) – A Pyro prior distribution.

autoguide(*name*, *dist_constructor*)

Sets an autoguide for an existing parameter with name `name` (mimic the behavior of module *pyro.infer.autoguide*).

Note: *dist_constructor* should be one of *Delta*, *Normal*, and *MultivariateNormal*. More distribution constructor will be supported in the future if needed.

Parameters

- **name** (*str*) – Name of the parameter.
- **dist_constructor** – A `Distribution` constructor.

set_mode(*mode*)

Sets `mode` of this object to be able to use its parameters in stochastic functions. If `mode="model"`, a parameter will get its value from its prior. If `mode="guide"`, the value will be drawn from its guide.

Note: This method automatically sets `mode` for submodules which belong to *Parameterized* class.

Parameters **mode** (*str*) – Either "model" or "guide".

mode

18.1 Models

18.1.1 GPModel

class GPModel(*X*, *y*, *kernel*, *mean_function=None*, *jitter=1e-06*)

Bases: *pyro.contrib.gp.parameterized.Parameterized*

Base class for Gaussian Process models.

The core of a Gaussian Process is a covariance function k which governs the similarity between input points. Given k, we can establish a distribution over functions f by a multivarite normal distribution

$$p(f(X)) = \mathcal{N}(0, k(X, X)),$$

where X is any set of input points and $k(X, X)$ is a covariance matrix whose entries are outputs $k(x, z)$ of k over input pairs (x, z). This distribution is usually denoted by

$$f \sim \mathcal{GP}(0, k).$$

Note: Generally, beside a covariance matrix k, a Gaussian Process can also be specified by a mean function m (which is a zero-value function by default). In that case, its distribution will be

$$p(f(X)) = \mathcal{N}(m(X), k(X, X)).$$

Gaussian Process models are `Parameterized` subclasses. So its parameters can be learned, set priors, or fixed by using corresponding methods from `Parameterized`. A typical way to define a Gaussian Process model is

```
>>> X = torch.tensor([[1., 5, 3], [4, 3, 7]])
>>> y = torch.tensor([2., 1])
>>> kernel = gp.kernels.RBF(input_dim=3)
>>> kernel.variance = pyro.nn.PyroSample(dist.Uniform(torch.tensor(0.5), torch.
↪tensor(1.5)))
>>> kernel.lengthscale = pyro.nn.PyroSample(dist.Uniform(torch.tensor(1.0), torch.
↪tensor(3.0)))
>>> gpr = gp.models.GPRegression(X, y, kernel)
```

There are two ways to train a Gaussian Process model:

- Using an MCMC algorithm (in module `pyro.infer.mcmc`) on *model()* to get posterior samples for the Gaussian Process's parameters. For example:

```
>>> hmc_kernel = HMC(gpr.model)
>>> mcmc = MCMC(hmc_kernel, num_samples=10)
>>> mcmc.run()
>>> ls_name = "kernel.lengthscale"
>>> posterior_ls = mcmc.get_samples()[ls_name]
```

- Using a variational inference on the pair *model()*, *guide()*:

```
>>> optimizer = torch.optim.Adam(gpr.parameters(), lr=0.01)
>>> loss_fn = pyro.infer.TraceMeanField_ELBO().differentiable_loss
>>>
>>> for i in range(1000):
...     svi.step()  # doctest: +SKIP
...     optimizer.zero_grad()
...     loss = loss_fn(gpr.model, gpr.guide)  # doctest: +SKIP
...     loss.backward()  # doctest: +SKIP
...     optimizer.step()
```

To give a prediction on new dataset, simply use *forward()* like any PyTorch `torch.nn.Module`:

```
>>> Xnew = torch.tensor([[2., 3, 1]])
>>> f_loc, f_cov = gpr(Xnew, full_cov=True)
```

Reference:

[1] *Gaussian Processes for Machine Learning*, Carl E. Rasmussen, Christopher K. I. Williams

Parameters

- **X** (*torch.Tensor*) – A input data for training. Its first dimension is the number of data points.
- **y** (*torch.Tensor*) – An output data for training. Its last dimension is the number of data points.
- **kernel** (*Kernel*) – A Pyro kernel object, which is the covariance function k.
- **mean_function** (*callable*) – An optional mean function m of this Gaussian process. By default, we use zero mean.

- **jitter** (*float*) – A small positive term which is added into the diagonal part of a covariance matrix to help stablize its Cholesky decomposition.

model()
A "model" stochastic function. If `self.y` is `None`, this method returns mean and variance of the Gaussian Process prior.

guide()
A "guide" stochastic function to be used in variational inference methods. It also gives posterior information to the method *forward()* for prediction.

forward(*Xnew*, *full_cov=False*)
Computes the mean and covariance matrix (or variance) of Gaussian Process posterior on a test input data X_{new}:

$$p(f^* \mid X_{new}, X, y, k, \theta),$$

where θ are parameters of this model.

Note: Model's parameters θ together with kernel's parameters have been learned from a training procedure (MCMC or SVI).

Parameters

- **Xnew** (*torch.Tensor*) – A input data for testing. Note that `Xnew.shape[1:]` must be the same as `X.shape[1:]`.
- **full_cov** (*bool*) – A flag to decide if we want to predict full covariance matrix or just variance.

Returns loc and covariance matrix (or variance) of $p(f^*(X_{new}))$

Return type tuple(torch.Tensor, torch.Tensor)

set_data(*X*, *y=None*)
Sets data for Gaussian Process models.

Some examples to utilize this method are:

- Batch training on a sparse variational model:

```
>>> Xu = torch.tensor([[1., 0, 2]])  # inducing input
>>> likelihood = gp.likelihoods.Gaussian()
>>> vsgp = gp.models.VariationalSparseGP(X, y, kernel, Xu, likelihood)
>>> optimizer = torch.optim.Adam(vsgp.parameters(), lr=0.01)
>>> loss_fn = pyro.infer.TraceMeanField_ELBO().differentiable_loss
>>> batched_X, batched_y = X.split(split_size=10), y.split(split_size=10)
>>> for Xi, yi in zip(batched_X, batched_y):
...     optimizer.zero_grad()
...     vsgp.set_data(Xi, yi)
...     svi.step()  # doctest: +SKIP
...     loss = loss_fn(vsgp.model, vsgp.guide)  # doctest: +SKIP
...     loss.backward()  # doctest: +SKIP
...     optimizer.step()
```

- Making a two-layer Gaussian Process stochastic function:

```
>>> gpr1 = gp.models.GPRegression(X, None, kernel)
>>> Z, _ = gpr1.model()
>>> gpr2 = gp.models.GPRegression(Z, y, kernel)
>>> def two_layer_model():
...     Z, _ = gpr1.model()
...     gpr2.set_data(Z, y)
...     return gpr2.model()
```

References:

[1] *Scalable Variational Gaussian Process Classification*, James Hensman, Alexander G. de G. Matthews, Zoubin Ghahramani

[2] *Deep Gaussian Processes*, Andreas C. Damianou, Neil D. Lawrence

Parameters

- **X** (*torch.Tensor*) – A input data for training. Its first dimension is the number of data points.
- **y** (*torch.Tensor*) – An output data for training. Its last dimension is the number of data points.

18.1.2 GPRegression

class GPRegression(*X*, *y*, *kernel*, *noise=None*, *mean_function=None*, *jitter=1e-06*)

Bases: *pyro.contrib.gp.models.model.GPModel*

Gaussian Process Regression model.

The core of a Gaussian Process is a covariance function k which governs the similarity between input points. Given k, we can establish a distribution over functions f by a multivarite normal distribution

$$p(f(X)) = \mathcal{N}(0, k(X, X)),$$

where X is any set of input points and $k(X, X)$ is a covariance matrix whose entries are outputs $k(x, z)$ of k over input pairs (x, z). This distribution is usually denoted by

$$f \sim \mathcal{GP}(0, k).$$

Note: Generally, beside a covariance matrix k, a Gaussian Process can also be specified by a mean function m (which is a zero-value function by default). In that case, its distribution will be

$$p(f(X)) = \mathcal{N}(m(X), k(X, X)).$$

Given inputs X and their noisy observations y, the Gaussian Process Regression model takes the form

$$f \sim \mathcal{GP}(0, k(X, X)),$$
$$y \sim f + \epsilon,$$

where ϵ is Gaussian noise.

Note: This model has $\mathcal{O}(N^3)$ complexity for training, $\mathcal{O}(N^3)$ complexity for testing. Here, N is the number of train inputs.

Reference:

[1] *Gaussian Processes for Machine Learning*, Carl E. Rasmussen, Christopher K. I. Williams

Parameters

- **X** (*torch.Tensor*) – A input data for training. Its first dimension is the number of data points.
- **y** (*torch.Tensor*) – An output data for training. Its last dimension is the number of data points.
- **kernel** (*Kernel*) – A Pyro kernel object, which is the covariance function k.
- **noise** (*torch.Tensor*) – Variance of Gaussian noise of this model.
- **mean_function** (*callable*) – An optional mean function m of this Gaussian process. By default, we use zero mean.
- **jitter** (*float*) – A small positive term which is added into the diagonal part of a covariance matrix to help stablize its Cholesky decomposition.

model()

guide()

forward(*Xnew*, *full_cov=False*, *noiseless=True*)

Computes the mean and covariance matrix (or variance) of Gaussian Process posterior on a test input data X_{new}:

$$p(f^* \mid X_{new}, X, y, k, \epsilon) = \mathcal{N}(loc, cov).$$

Note: The noise parameter `noise` (ϵ) together with kernel's parameters have been learned from a training procedure (MCMC or SVI).

Parameters

- **Xnew** (*torch.Tensor*) – A input data for testing. Note that `Xnew.shape[1:]` must be the same as `self.X.shape[1:]`.
- **full_cov** (*bool*) – A flag to decide if we want to predict full covariance matrix or just variance.
- **noiseless** (*bool*) – A flag to decide if we want to include noise in the prediction output or not.

Returns loc and covariance matrix (or variance) of $p(f^*(X_{new}))$

Return type tuple(torch.Tensor, torch.Tensor)

iter_sample(*noiseless=True*)

Iteratively constructs a sample from the Gaussian Process posterior.

Recall that at test input points X_{new}, the posterior is multivariate Gaussian distributed with mean and covariance matrix given by *forward()*.

This method samples lazily from this multivariate Gaussian. The advantage of this approach is that later query points can depend upon earlier ones. Particularly useful when the querying is to be done by an optimisation routine.

Note: The noise parameter `noise` (ϵ) together with kernel's parameters have been learned from a training procedure (MCMC or SVI).

Parameters **noiseless** (*bool*) – A flag to decide if we want to add sampling noise to the samples beyond the noise inherent in the GP posterior.

Returns sampler

Return type function

18.1.3 SparseGPRegression

class SparseGPRegression(*X*, *y*, *kernel*, *Xu*, *noise=None*, *mean_function=None*, *approx=None*, *jitter=1e-06*)

Bases: *pyro.contrib.gp.models.model.GPModel*

Sparse Gaussian Process Regression model.

In *GPRegression* model, when the number of input data X is large, the covariance matrix $k(X, X)$ will require a lot of computational steps to compute its inverse (for log likelihood and for prediction). By introducing an additional inducing-input parameter X_u, we can reduce computational cost by approximate $k(X, X)$ by a low-rank Nyström approximation Q (see reference [1]), where

$$Q = k(X, X_u)k(X, X)^{-1}k(X_u, X).$$

Given inputs X, their noisy observations y, and the inducing-input parameters X_u, the model takes the form:

$$\begin{aligned} u &\sim \mathcal{GP}(0, k(X_u, X_u)), \\ f &\sim q(f \mid X, X_u) = \mathbb{E}_{p(u)} q(f \mid X, X_u, u), \\ y &\sim f + \epsilon, \end{aligned}$$

where ϵ is Gaussian noise and the conditional distribution $q(f \mid X, X_u, u)$ is an approximation of

$$p(f \mid X, X_u, u) = \mathcal{N}(m, k(X, X) - Q),$$

whose terms m and $k(X, X) - Q$ is derived from the joint multivariate normal distribution:

$$[f, u] \sim \mathcal{GP}(0, k([X, X_u], [X, X_u])).$$

This class implements three approximation methods:

- Deterministic Training Conditional (DTC):

$$q(f \mid X, X_u, u) = \mathcal{N}(m, 0),$$

  which in turns will imply

$$f \sim \mathcal{N}(0, Q).$$

- Fully Independent Training Conditional (FITC):

$$q(f \mid X, X_u, u) = \mathcal{N}(m, diag(k(X, X) - Q)),$$

which in turns will correct the diagonal part of the approximation in DTC:

$$f \sim \mathcal{N}(0, Q + diag(k(X, X) - Q)).$$

- Variational Free Energy (VFE), which is similar to DTC but has an additional *trace_term* in the model's log likelihood. This additional term makes "VFE" equivalent to the variational approach in `SparseVariationalGP` (see reference [2]).

Note: This model has $\mathcal{O}(NM^2)$ complexity for training, $\mathcal{O}(NM^2)$ complexity for testing. Here, N is the number of train inputs, M is the number of inducing inputs.

References:

[1] *A Unifying View of Sparse Approximate Gaussian Process Regression*, Joaquin Quiñonero-Candela, Carl E. Rasmussen

[2] *Variational learning of inducing variables in sparse Gaussian processes*, Michalis Titsias

Parameters

- **X** (*torch.Tensor*) – A input data for training. Its first dimension is the number of data points.
- **y** (*torch.Tensor*) – An output data for training. Its last dimension is the number of data points.
- **kernel** (*Kernel*) – A Pyro kernel object, which is the covariance function k.
- **Xu** (*torch.Tensor*) – Initial values for inducing points, which are parameters of our model.
- **noise** (*torch.Tensor*) – Variance of Gaussian noise of this model.
- **mean_function** (*callable*) – An optional mean function m of this Gaussian process. By default, we use zero mean.
- **approx** (*str*) – One of approximation methods: "DTC", "FITC", and "VFE" (default).
- **jitter** (*float*) – A small positive term which is added into the diagonal part of a covariance matrix to help stablize its Cholesky decomposition.
- **name** (*str*) – Name of this model.

model()

guide()

forward(*Xnew*, *full_cov=False*, *noiseless=True*)

Computes the mean and covariance matrix (or variance) of Gaussian Process posterior on a test input data X_{new}:

$$p(f^* \mid X_{new}, X, y, k, X_u, \epsilon) = \mathcal{N}(loc, cov).$$

Note: The noise parameter `noise` (ϵ), the inducing-point parameter `Xu`, together with kernel's parameters have been learned from a training procedure (MCMC or SVI).

Parameters

- **Xnew** (*torch.Tensor*) – A input data for testing. Note that `Xnew.shape[1:]` must be the same as `self.X.shape[1:]`.
- **full_cov** (*bool*) – A flag to decide if we want to predict full covariance matrix or just variance.
- **noiseless** (*bool*) – A flag to decide if we want to include noise in the prediction output or not.

Returns loc and covariance matrix (or variance) of $p(f^*(X_{new}))$

Return type tuple(torch.Tensor, torch.Tensor)

18.1.4 VariationalGP

class VariationalGP(*X*, *y*, *kernel*, *likelihood*, *mean_function=None*, *latent_shape=None*, *whiten=False*, *jitter=1e-06*)

Bases: *pyro.contrib.gp.models.model.GPModel*

Variational Gaussian Process model.

This model deals with both Gaussian and non-Gaussian likelihoods. Given inputs X and their noisy observations y, the model takes the form

$$f \sim \mathcal{GP}(0, k(X, X)),$$
$$y \sim p(y) = p(y \mid f)p(f),$$

where $p(y \mid f)$ is the likelihood.

We will use a variational approach in this model by approximating $q(f)$ to the posterior $p(f \mid y)$. Precisely, $q(f)$ will be a multivariate normal distribution with two parameters `f_loc` and `f_scale_tril`, which will be learned during a variational inference process.

Note: This model can be seen as a special version of `SparseVariationalGP` model with $X_u = X$.

Note: This model has $\mathcal{O}(N^3)$ complexity for training, $\mathcal{O}(N^3)$ complexity for testing. Here, N is the number of train inputs. Size of variational parameters is $\mathcal{O}(N^2)$.

Parameters

- **X** (*torch.Tensor*) – A input data for training. Its first dimension is the number of data points.
- **y** (*torch.Tensor*) – An output data for training. Its last dimension is the number of data points.
- **kernel** (*Kernel*) – A Pyro kernel object, which is the covariance function k.
- **Likelihood likelihood** (*likelihood*) – A likelihood object.

- **mean_function** (*callable*) – An optional mean function m of this Gaussian process. By default, we use zero mean.
- **latent_shape** (*torch.Size*) – Shape for latent processes (*batch_shape* of $q(f)$). By default, it equals to output batch shape `y.shape[:-1]`. For the multi-class classification problems, `latent_shape[-1]` should corresponse to the number of classes.
- **whiten** (*bool*) – A flag to tell if variational parameters `f_loc` and `f_scale_tril` are transformed by the inverse of `Lff`, where `Lff` is the lower triangular decomposition of $kernel(X, X)$. Enable this flag will help optimization.
- **jitter** (*float*) – A small positive term which is added into the diagonal part of a covariance matrix to help stablize its Cholesky decomposition.

model()

guide()

forward(*Xnew*, *full_cov=False*)

Computes the mean and covariance matrix (or variance) of Gaussian Process posterior on a test input data X_{new}:

$$p(f^* \mid X_{new}, X, y, k, f_{loc}, f_{scale\_tril}) = \mathcal{N}(loc, cov).$$

Note: Variational parameters `f_loc`, `f_scale_tril`, together with kernel's parameters have been learned from a training procedure (MCMC or SVI).

Parameters

- **Xnew** (*torch.Tensor*) – A input data for testing. Note that `Xnew.shape[1:]` must be the same as `self.X.shape[1:]`.
- **full_cov** (*bool*) – A flag to decide if we want to predict full covariance matrix or just variance.

Returns loc and covariance matrix (or variance) of $p(f^*(X_{new}))$

Return type tuple(torch.Tensor, torch.Tensor)

18.1.5 VariationalSparseGP

class VariationalSparseGP(*X*, *y*, *kernel*, *Xu*, *likelihood*, *mean_function=None*, *latent_shape=None*, *num_data=None*, *whiten=False*, *jitter=1e-06*)

Bases: *pyro.contrib.gp.models.model.GPModel*

Variational Sparse Gaussian Process model.

In *VariationalGP* model, when the number of input data X is large, the covariance matrix $k(X, X)$ will require a lot of computational steps to compute its inverse (for log likelihood and for prediction). This model introduces an additional inducing-input parameter X_u to solve that problem. Given inputs X, their noisy observations y, and the inducing-input parameters X_u, the model takes the form:

$$[f, u] \sim \mathcal{GP}(0, k([X, X_u], [X, X_u])),$$
$$y \sim p(y) = p(y \mid f)p(f),$$

where $p(y \mid f)$ is the likelihood.

We will use a variational approach in this model by approximating $q(f, u)$ to the posterior $p(f, u \mid y)$. Precisely, $q(f) = p(f \mid u)q(u)$, where $q(u)$ is a multivariate normal distribution with two parameters `u_loc` and `u_scale_tril`, which will be learned during a variational inference process.

Note: This model can be learned using MCMC method as in reference [2]. See also *GPModel*.

Note: This model has $\mathcal{O}(NM^2)$ complexity for training, $\mathcal{O}(M^3)$ complexity for testing. Here, N is the number of train inputs, M is the number of inducing inputs. Size of variational parameters is $\mathcal{O}(M^2)$.

References:

[1] *Scalable variational Gaussian process classification*, James Hensman, Alexander G. de G. Matthews, Zoubin Ghahramani

[2] *MCMC for Variationally Sparse Gaussian Processes*, James Hensman, Alexander G. de G. Matthews, Maurizio Filippone, Zoubin Ghahramani

Parameters

- **X** (*torch.Tensor*) – A input data for training. Its first dimension is the number of data points.
- **y** (*torch.Tensor*) – An output data for training. Its last dimension is the number of data points.
- **kernel** (*Kernel*) – A Pyro kernel object, which is the covariance function k.
- **Xu** (*torch.Tensor*) – Initial values for inducing points, which are parameters of our model.
- **Likelihood likelihood** (*likelihood*) – A likelihood object.
- **mean_function** (*callable*) – An optional mean function m of this Gaussian process. By default, we use zero mean.
- **latent_shape** (*torch.Size*) – Shape for latent processes (*batch_shape* of $q(u)$). By default, it equals to output batch shape `y.shape[:-1]`. For the multi-class classification problems, `latent_shape[-1]` should corresponse to the number of classes.
- **num_data** (*int*) – The size of full training dataset. It is useful for training this model with mini-batch.
- **whiten** (*bool*) – A flag to tell if variational parameters `u_loc` and `u_scale_tril` are transformed by the inverse of `Luu`, where `Luu` is the lower triangular decomposition of $kernel(X_u, X_u)$. Enable this flag will help optimization.
- **jitter** (*float*) – A small positive term which is added into the diagonal part of a covariance matrix to help stablize its Cholesky decomposition.

model()

guide()

forward(*Xnew*, *full_cov=False*)

Computes the mean and covariance matrix (or variance) of Gaussian Process posterior on a test input data X_{new}:

$$p(f^* \mid X_{new}, X, y, k, X_u, u_{loc}, u_{scale\_tril}) = \mathcal{N}(loc, cov).$$

Note: Variational parameters `u_loc`, `u_scale_tril`, the inducing-point parameter `Xu`, together with kernel's parameters have been learned from a training procedure (MCMC or SVI).

Parameters

- **Xnew** (*torch.Tensor*) – A input data for testing. Note that `Xnew.shape[1:]` must be the same as `self.X.shape[1:]`.
- **full_cov** (*bool*) – A flag to decide if we want to predict full covariance matrix or just variance.

Returns loc and covariance matrix (or variance) of $p(f^*(X_{new}))$

Return type tuple(torch.Tensor, torch.Tensor)

18.1.6 GPLVM

class GPLVM(*base_model*)

Bases: *pyro.contrib.gp.parameterized.Parameterized*

Gaussian Process Latent Variable Model (GPLVM) model.

GPLVM is a Gaussian Process model with its train input data is a latent variable. This model is useful for dimensional reduction of high dimensional data. Assume the mapping from low dimensional latent variable to is a Gaussian Process instance. Then the high dimensional data will play the role of train output `y` and our target is to learn latent inputs which best explain `y`. For the purpose of dimensional reduction, latent inputs should have lower dimensions than `y`.

We follows reference [1] to put a unit Gaussian prior to the input and approximate its posterior by a multivariate normal distribution with two variational parameters: `X_loc` and `X_scale_tril`.

For example, we can do dimensional reduction on Iris dataset as follows:

```
>>> # With y as the 2D Iris data of shape 150x4 and we want to reduce its␣
↪dimension
>>> # to a tensor X of shape 150x2, we will use GPLVM.
```

```
>>> # First, define the initial values for X parameter:
>>> X_init = torch.zeros(150, 2)
>>> # Then, define a Gaussian Process model with input X_init and output␣
↪y:
>>> kernel = gp.kernels.RBF(input_dim=2, lengthscale=torch.ones(2))
>>> Xu = torch.zeros(20, 2)  # initial inducing inputs of sparse model
>>> gpmodule = gp.models.SparseGPRegression(X_init, y, kernel, Xu)
>>> # Finally, wrap gpmodule by GPLVM, optimize, and get the "learned"␣
↪mean of X:
>>> gplvm = gp.models.GPLVM(gpmodule)
>>> gp.util.train(gplvm)  # doctest: +SKIP
>>> X = gplvm.X
```

Reference:

[1] Bayesian Gaussian Process Latent Variable Model Michalis K. Titsias, Neil D. Lawrence

Parameters **base_model** (GPModel) – A Pyro Gaussian Process model object. Note that `base_model.X` will be the initial value for the variational parameter `X_loc`.

model()

guide()

forward(***kwargs*)
Forward method has the same signal as its `base_model`. Note that the train input data of `base_model` is sampled from GPLVM.

18.2 Kernels

18.2.1 Kernel

class Kernel(*input_dim*, *active_dims=None*)
Bases: *pyro.contrib.gp.parameterized.Parameterized*

Base class for kernels used in this Gaussian Process module.

Every inherited class should implement a *forward()* pass which takes inputs X, Z and returns their covariance matrix.

To construct a new kernel from the old ones, we can use methods `add()`, `mul()`, `exp()`, `warp()`, `vertical_scale()`.

References:

[1] *Gaussian Processes for Machine Learning*, Carl E. Rasmussen, Christopher K. I. Williams

Parameters

- **input_dim** (*int*) – Number of feature dimensions of inputs.
- **variance** (*torch.Tensor*) – Variance parameter of this kernel.
- **active_dims** (*list*) – List of feature dimensions of the input which the kernel acts on.

forward(*X*, *Z=None*, *diag=False*)
Calculates covariance matrix of inputs on active dimensionals.

Parameters

- **X** (*torch.Tensor*) – A 2D tensor with shape $N \times input\_dim$.
- **Z** (*torch.Tensor*) – An (optional) 2D tensor with shape $M \times input\_dim$.
- **diag** (*bool*) – A flag to decide if we want to return full covariance matrix or just its diagonal part.

Returns covariance matrix of X and Z with shape $N \times M$

Return type torch.Tensor

18.2.2 Brownian

class Brownian(*input_dim*, *variance=None*, *active_dims=None*)
Bases: `pyro.contrib.gp.kernels.kernel.Kernel`

This kernel correponds to a two-sided Brownion motion (Wiener process):

$$k(x,z) = \begin{cases} \sigma^2 \min(|x|,|z|), & \text{if } x \cdot z \geq 0 \\ 0, & \text{otherwise.} \end{cases}$$

Note that the input dimension of this kernel must be 1.

Reference:

[1] *Theory and Statistical Applications of Stochastic Processes*, Yuliya Mishura, Georgiy Shevchenko

forward(*X*, *Z=None*, *diag=False*)

18.2.3 Combination

class Combination(*kern0*, *kern1*)

Bases: pyro.contrib.gp.kernels.kernel.Kernel

Base class for kernels derived from a combination of kernels.

Parameters

- **kern0** (Kernel) – First kernel to combine.
- **kern1** (Kernel *or* *numbers.Number*) – Second kernel to combine.

18.2.4 Constant

class Constant(*input_dim*, *variance=None*, *active_dims=None*)

Bases: pyro.contrib.gp.kernels.kernel.Kernel

Implementation of Constant kernel:

$$k(x, z) = \sigma^2.$$

forward(*X*, *Z=None*, *diag=False*)

18.2.5 Coregionalize

class Coregionalize(*input_dim*, *rank=None*, *components=None*, *diagonal=None*, *active_dims=None*)

Bases: pyro.contrib.gp.kernels.kernel.Kernel

A kernel for the linear model of coregionalization $k(x, z) = x^T(WW^T + D)z$ where W is an `input_dim`-by-`rank` matrix and typically `rank < input_dim`, and `D` is a diagonal matrix.

This generalizes the `Linear` kernel to multiple features with a low-rank-plus-diagonal weight matrix. The typical use case is for modeling correlations among outputs of a multi-output GP, where outputs are coded as distinct data points with one-hot coded features denoting which output each datapoint represents.

If only `rank` is specified, the kernel `(W W^T + D)` will be randomly initialized to a matrix with expected value the identity matrix.

References:

[1] Mauricio A. Alvarez, Lorenzo Rosasco, Neil D. Lawrence (2012) Kernels for Vector-Valued Functions: a Review

Parameters

- **input_dim** (*int*) – Number of feature dimensions of inputs.
- **rank** (*int*) – Optional rank. This is only used if `components` is unspecified. If neigher `rank` nor `components` is specified, then `rank` defaults to `input_dim`.

- **components** (*torch.Tensor*) – An optional `(input_dim, rank)` shaped matrix that maps features to `rank`-many components. If unspecified, this will be randomly initialized.
- **diagonal** (*torch.Tensor*) – An optional vector of length `input_dim`. If unspecified, this will be set to constant `0.5`.
- **active_dims** (*list*) – List of feature dimensions of the input which the kernel acts on.
- **name** (*str*) – Name of the kernel.

forward(*X*, *Z=None*, *diag=False*)

18.2.6 Cosine

class Cosine(*input_dim*, *variance=None*, *lengthscale=None*, *active_dims=None*)

Bases: `pyro.contrib.gp.kernels.isotropic.Isotropy`

Implementation of Cosine kernel:

$$k(x,z) = \sigma^2 \cos\left(\frac{|x-z|}{l}\right).$$

Parameters **lengthscale** (*torch.Tensor*) – Length-scale parameter of this kernel.

forward(*X*, *Z=None*, *diag=False*)

18.2.7 DotProduct

class DotProduct(*input_dim*, *variance=None*, *active_dims=None*)

Bases: `pyro.contrib.gp.kernels.kernel.Kernel`

Base class for kernels which are functions of $x \cdot z$.

18.2.8 Exponent

class Exponent(*kern*)

Bases: `pyro.contrib.gp.kernels.kernel.Transforming`

Creates a new kernel according to

$$k_{new}(x,z) = \exp(k(x,z)).$$

forward(*X*, *Z=None*, *diag=False*)

18.2.9 Exponential

class Exponential(*input_dim*, *variance=None*, *lengthscale=None*, *active_dims=None*)

Bases: `pyro.contrib.gp.kernels.isotropic.Isotropy`

Implementation of Exponential kernel:

$$k(x,z) = \sigma^2 \exp\left(-\frac{|x-z|}{l}\right).$$

forward(*X*, *Z=None*, *diag=False*)

18.2.10 Isotropy

class Isotropy(*input_dim*, *variance=None*, *lengthscale=None*, *active_dims=None*)
Bases: pyro.contrib.gp.kernels.kernel.Kernel

Base class for a family of isotropic covariance kernels which are functions of the distance $|x - z|/l$, where l is the length-scale parameter.

By default, the parameter `lengthscale` has size 1. To use the isotropic version (different lengthscale for each dimension), make sure that `lengthscale` has size equal to `input_dim`.

Parameters **lengthscale** (*torch.Tensor*) – Length-scale parameter of this kernel.

18.2.11 Linear

class Linear(*input_dim*, *variance=None*, *active_dims=None*)
Bases: pyro.contrib.gp.kernels.dot_product.DotProduct

Implementation of Linear kernel:

$$k(x, z) = \sigma^2 x \cdot z.$$

Doing Gaussian Process regression with linear kernel is equivalent to doing a linear regression.

Note: Here we implement the homogeneous version. To use the inhomogeneous version, consider using *Polynomial* kernel with `degree=1` or making a *Sum* with a *Constant* kernel.

---

forward(*X*, *Z=None*, *diag=False*)

18.2.12 Matern32

class Matern32(*input_dim*, *variance=None*, *lengthscale=None*, *active_dims=None*)
Bases: pyro.contrib.gp.kernels.isotropic.Isotropy

Implementation of Matern32 kernel:

$$k(x, z) = \sigma^2 \left(1 + \sqrt{3} \times \frac{|x-z|}{l}\right) \exp\left(-\sqrt{3} \times \frac{|x-z|}{l}\right).$$

forward(*X*, *Z=None*, *diag=False*)

18.2.13 Matern52

class Matern52(*input_dim*, *variance=None*, *lengthscale=None*, *active_dims=None*)
Bases: pyro.contrib.gp.kernels.isotropic.Isotropy

Implementation of Matern52 kernel:

$$k(x, z) = \sigma^2 \left(1 + \sqrt{5} \times \frac{|x-z|}{l} + \frac{5}{3} \times \frac{|x-z|^2}{l^2}\right) \exp\left(-\sqrt{5} \times \frac{|x-z|}{l}\right).$$

forward(*X*, *Z=None*, *diag=False*)

18.2.14 Periodic

class Periodic(*input_dim*, *variance=None*, *lengthscale=None*, *period=None*, *active_dims=None*)
Bases: pyro.contrib.gp.kernels.kernel.Kernel

Implementation of Periodic kernel:

$$k(x,z) = \sigma^2 \exp\left(-2 \times \frac{\sin^2(\pi(x-z)/p)}{l^2}\right),$$

where p is the period parameter.

References:

[1] *Introduction to Gaussian processes*, David J.C. MacKay

Parameters

- **lengthscale** (*torch.Tensor*) – Length scale parameter of this kernel.
- **period** (*torch.Tensor*) – Period parameter of this kernel.

forward(*X*, *Z=None*, *diag=False*)

18.2.15 Polynomial

class Polynomial(*input_dim*, *variance=None*, *bias=None*, *degree=1*, *active_dims=None*)
Bases: pyro.contrib.gp.kernels.dot_product.DotProduct

Implementation of Polynomial kernel:

$$k(x,z) = \sigma^2(\text{bias} + x \cdot z)^d.$$

Parameters

- **bias** (*torch.Tensor*) – Bias parameter of this kernel. Should be positive.
- **degree** (*int*) – Degree d of the polynomial.

forward(*X*, *Z=None*, *diag=False*)

18.2.16 Product

class Product(*kern0*, *kern1*)
Bases: pyro.contrib.gp.kernels.kernel.Combination

Returns a new kernel which acts like a product/tensor product of two kernels. The second kernel can be a constant.

forward(*X*, *Z=None*, *diag=False*)

18.2.17 RBF

class RBF(*input_dim*, *variance=None*, *lengthscale=None*, *active_dims=None*)
Bases: pyro.contrib.gp.kernels.isotropic.Isotropy

Implementation of Radial Basis Function kernel:

$$k(x,z) = \sigma^2 \exp\left(-0.5 \times \frac{|x-z|^2}{l^2}\right).$$

Note: This kernel also has name *Squared Exponential* in literature.

forward(*X*, *Z=None*, *diag=False*)

18.2.18 RationalQuadratic

class RationalQuadratic(*input_dim*, *variance=None*, *lengthscale=None*, *scale_mixture=None*, *active_dims=None*)

Bases: pyro.contrib.gp.kernels.isotropic.Isotropy

Implementation of RationalQuadratic kernel:

$$k(x,z) = \sigma^2 \left(1 + 0.5 \times \frac{|x-z|^2}{\alpha l^2}\right)^{-\alpha}.$$

Parameters **scale_mixture** (*torch.Tensor*) – Scale mixture (α) parameter of this kernel. Should have size 1.

forward(*X*, *Z=None*, *diag=False*)

18.2.19 Sum

class Sum(*kern0*, *kern1*)

Bases: pyro.contrib.gp.kernels.kernel.Combination

Returns a new kernel which acts like a sum/direct sum of two kernels. The second kernel can be a constant.

forward(*X*, *Z=None*, *diag=False*)

18.2.20 Transforming

class Transforming(*kern*)

Bases: pyro.contrib.gp.kernels.kernel.Kernel

Base class for kernels derived from a kernel by some transforms such as warping, exponent, vertical scaling.

Parameters **kern** (*Kernel*) – The original kernel.

18.2.21 VerticalScaling

class VerticalScaling(*kern*, *vscaling_fn*)

Bases: pyro.contrib.gp.kernels.kernel.Transforming

Creates a new kernel according to

$$k_{new}(x,z) = f(x)k(x,z)f(z),$$

where f is a function.

Parameters **vscaling_fn** (*callable*) – A vertical scaling function f.

forward(*X*, *Z=None*, *diag=False*)

18.2.22 Warping

class Warping(*kern*, *iwarping_fn=None*, *owarping_coef=None*)
Bases: pyro.contrib.gp.kernels.kernel.Transforming

Creates a new kernel according to

$$k_{new}(x, z) = q(k(f(x), f(z))),$$

where f is an function and q is a polynomial with non-negative coefficients owarping_coef.

We can take advantage of f to combine a Gaussian Process kernel with a deep learning architecture. For example:

```
>>> linear = torch.nn.Linear(10, 3)
>>> # register its parameters to Pyro's ParamStore and wrap it by lambda
>>> # to call the primitive pyro.module each time we use the linear function
>>> pyro_linear_fn = lambda x: pyro.module("linear", linear)(x)
>>> kernel = gp.kernels.Matern52(input_dim=3, lengthscale=torch.ones(3))
>>> warped_kernel = gp.kernels.Warping(kernel, pyro_linear_fn)
```

Reference:

[1] *Deep Kernel Learning*, Andrew G. Wilson, Zhiting Hu, Ruslan Salakhutdinov, Eric P. Xing

Parameters

- **iwarping_fn** (*callable*) – An input warping function f.
- **owarping_coef** (*list*) – A list of coefficients of the output warping polynomial. These coefficients must be non-negative.

forward(*X*, *Z=None*, *diag=False*)

18.2.23 WhiteNoise

class WhiteNoise(*input_dim*, *variance=None*, *active_dims=None*)
Bases: pyro.contrib.gp.kernels.kernel.Kernel

Implementation of WhiteNoise kernel:

$$k(x, z) = \sigma^2 \delta(x, z),$$

where δ is a Dirac delta function.

forward(*X*, *Z=None*, *diag=False*)

18.3 Likelihoods

18.3.1 Likelihood

class Likelihood
Bases: *pyro.contrib.gp.parameterized.Parameterized*

Base class for likelihoods used in Gaussian Process.

Every inherited class should implement a forward pass which takes an input f and returns a sample y.

forward(*f_loc*, *f_var*, *y=None*)
Samples y given f_{loc}, f_{var}.

Parameters

- **f_loc** (*torch.Tensor*) – Mean of latent function output.
- **f_var** (*torch.Tensor*) – Variance of latent function output.
- **y** (*torch.Tensor*) – Training output tensor.

Returns a tensor sampled from likelihood

Return type torch.Tensor

18.3.2 Binary

class Binary(*response_function=None*)

Bases: pyro.contrib.gp.likelihoods.likelihood.Likelihood

Implementation of Binary likelihood, which is used for binary classification problems.

Binary likelihood uses *Bernoulli* distribution, so the output of `response_function` should be in range $(0, 1)$. By default, we use *sigmoid* function.

Parameters **response_function** (*callable*) – A mapping to correct domain for Binary likelihood.

forward(*f_loc*, *f_var*, *y=None*)

Samples y given f_{loc}, f_{var} according to

$$f \sim \mathbb{N}(f_{loc}, f_{var}),$$
$$y \sim \mathbb{B}(\text{response\_function}(f)).$$

Note: The log likelihood is estimated using Monte Carlo with 1 sample of f.

Parameters

- **f_loc** (*torch.Tensor*) – Mean of latent function output.
- **f_var** (*torch.Tensor*) – Variance of latent function output.
- **y** (*torch.Tensor*) – Training output tensor.

Returns a tensor sampled from likelihood

Return type torch.Tensor

18.3.3 Gaussian

class Gaussian(*variance=None*)

Bases: pyro.contrib.gp.likelihoods.likelihood.Likelihood

Implementation of Gaussian likelihood, which is used for regression problems.

Gaussian likelihood uses *Normal* distribution.

Parameters **variance** (*torch.Tensor*) – A variance parameter, which plays the role of `noise` in regression problems.

forward(*f_loc*, *f_var*, *y=None*)
Samples y given f_{loc}, f_{var} according to

$$y \sim \mathbb{N}\bowtie\diagdown\gg\partial\ll(f_{loc}, f_{var} + \epsilon),$$

where ϵ is the `variance` parameter of this likelihood.

Parameters

- **f_loc** (*torch.Tensor*) – Mean of latent function output.
- **f_var** (*torch.Tensor*) – Variance of latent function output.
- **y** (*torch.Tensor*) – Training output tensor.

Returns a tensor sampled from likelihood

Return type torch.Tensor

18.3.4 MultiClass

class MultiClass(*num_classes*, *response_function=None*)
Bases: `pyro.contrib.gp.likelihoods.likelihood.Likelihood`

Implementation of MultiClass likelihood, which is used for multi-class classification problems.

MultiClass likelihood uses *Categorical* distribution, so `response_function` should normalize its input's rightmost axis. By default, we use *softmax* function.

Parameters

- **num_classes** (*int*) – Number of classes for prediction.
- **response_function** (*callable*) – A mapping to correct domain for MultiClass likelihood.

forward(*f_loc*, *f_var*, *y=None*)
Samples y given f_{loc}, f_{var} according to

$$f \sim \mathbb{N}\bowtie\diagdown\gg\partial\ll(f_{loc}, f_{var}),$$
$$y \sim \mathbb{C}\partial\approx\eth\bowtie\diagdown\sqsupset\partial\ll(f).$$

Note: The log likelihood is estimated using Monte Carlo with 1 sample of f.

Parameters

- **f_loc** (*torch.Tensor*) – Mean of latent function output.
- **f_var** (*torch.Tensor*) – Variance of latent function output.
- **y** (*torch.Tensor*) – Training output tensor.

Returns a tensor sampled from likelihood

Return type torch.Tensor

18.3.5 Poisson

class Poisson(*response_function=None*)
Bases: pyro.contrib.gp.likelihoods.likelihood.Likelihood

Implementation of Poisson likelihood, which is used for count data.

Poisson likelihood uses the *Poisson* distribution, so the output of `response_function` should be positive. By default, we use `torch.exp()` as response function, corresponding to a log-Gaussian Cox process.

Parameters **response_function** (*callable*) – A mapping to positive real numbers.

forward(*f_loc*, *f_var*, *y=None*)
Samples y given f_{loc}, f_{var} according to

$$f \sim \mathbb{N}\bowtie\searrow\gtrdot\partial\lessdot(f_{loc}, f_{var}),$$
$$y \sim \mathbb{P}\bowtie\beth\sim\sim\bowtie\ltimes(\exp(f)).$$

Note: The log likelihood is estimated using Monte Carlo with 1 sample of f.

Parameters

- **f_loc** (*torch.Tensor*) – Mean of latent function output.
- **f_var** (*torch.Tensor*) – Variance of latent function output.
- **y** (*torch.Tensor*) – Training output tensor.

Returns a tensor sampled from likelihood

Return type torch.Tensor

18.4 Parameterized

class Parameterized
Bases: *pyro.nn.module.PyroModule*

A wrapper of *PyroModule* whose parameters can be set constraints, set priors.

By default, when we set a prior to a parameter, an auto Delta guide will be created. We can use the method *autoguide()* to setup other auto guides.

Example:

```
>>> class Linear(Parameterized):
...     def __init__(self, a, b):
...         super().__init__()
...         self.a = Parameter(a)
...         self.b = Parameter(b)
...
...     def forward(self, x):
...         return self.a * x + self.b
...
>>> linear = Linear(torch.tensor(1.), torch.tensor(0.))
>>> linear.a = PyroParam(torch.tensor(1.), constraints.positive)
>>> linear.b = PyroSample(dist.Normal(0, 1))
```

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```
>>> linear.autoguide("b", dist.Normal)
>>> assert "a_unconstrained" in dict(linear.named_parameters())
>>> assert "b_loc" in dict(linear.named_parameters())
>>> assert "b_scale_unconstrained" in dict(linear.named_parameters())
```

Note that by default, data of a parameter is a float `torch.Tensor` (unless we use `torch.set_default_tensor_type()` to change default tensor type). To cast these parameters to a correct data type or GPU device, we can call methods such as `double()` or `cuda()`. See `torch.nn.Module` for more information.

set_prior(*name*, *prior*)

Sets prior for a parameter.

Parameters

- **name** (*str*) – Name of the parameter.
- **prior** (*Distribution*) – A Pyro prior distribution.

autoguide(*name*, *dist_constructor*)

Sets an autoguide for an existing parameter with name `name` (mimic the behavior of module *pyro.infer.autoguide*).

Note: *dist_constructor* should be one of *Delta*, *Normal*, and *MultivariateNormal*. More distribution constructor will be supported in the future if needed.

Parameters

- **name** (*str*) – Name of the parameter.
- **dist_constructor** – A `Distribution` constructor.

set_mode(*mode*)

Sets `mode` of this object to be able to use its parameters in stochastic functions. If `mode="model"`, a parameter will get its value from its prior. If `mode="guide"`, the value will be drawn from its guide.

Note: This method automatically sets `mode` for submodules which belong to *Parameterized* class.

Parameters **mode** (*str*) – Either "model" or "guide".

mode

18.5 Util

conditional(*Xnew*, *X*, *kernel*, *f_loc*, *f_scale_tril=None*, *Lff=None*, *full_cov=False*, *whiten=False*, *jitter=1e-06*)

Given X_{new}, predicts loc and covariance matrix of the conditional multivariate normal distribution

$$p(f^*(X_{new}) \mid X, k, f_{loc}, f_{scale\_tril}).$$

Here `f_loc` and `f_scale_tril` are variation parameters of the variational distribution

$$q(f \mid f_{loc}, f_{scale\_tril}) \sim p(f|X, y),$$

where f is the function value of the Gaussian Process given input X

$$p(f(X)) \sim \mathcal{N}(0, k(X, X))$$

and y is computed from f by some likelihood function $p(y|f)$.

In case `f_scale_tril=None`, we consider $f = f_{loc}$ and computes

$$p(f^*(X_{new}) \mid X, k, f).$$

In case `f_scale_tril` is not `None`, we follow the derivation from reference [1]. For the case `f_scale_tril=None`, we follow the popular reference [2].

References:

[1] Sparse GPs: approximate the posterior, not the model

[2] *Gaussian Processes for Machine Learning*, Carl E. Rasmussen, Christopher K. I. Williams

Parameters

- **Xnew** (*torch.Tensor*) – A new input data.
- **X** (*torch.Tensor*) – An input data to be conditioned on.
- **kernel** (*Kernel*) – A Pyro kernel object.
- **f_loc** (*torch.Tensor*) – Mean of $q(f)$. In case `f_scale_tril=None`, $f_{loc} = f$.
- **f_scale_tril** (*torch.Tensor*) – Lower triangular decomposition of covariance matrix of $q(f)$'s .
- **Lff** (*torch.Tensor*) – Lower triangular decomposition of $kernel(X, X)$ (optional).
- **full_cov** (*bool*) – A flag to decide if we want to return full covariance matrix or just variance.
- **whiten** (*bool*) – A flag to tell if `f_loc` and `f_scale_tril` are already transformed by the inverse of `Lff`.
- **jitter** (*float*) – A small positive term which is added into the diagonal part of a covariance matrix to help stablize its Cholesky decomposition.

Returns loc and covariance matrix (or variance) of $p(f^*(X_{new}))$

Return type tuple(torch.Tensor, torch.Tensor)

train(*gpmodule*, *optimizer=None*, *loss_fn=None*, *retain_graph=None*, *num_steps=1000*)

A helper to optimize parameters for a GP module.

Parameters

- **gpmodule** (*GPModel*) – A GP module.
- **optimizer** (*Optimizer*) – A PyTorch optimizer instance. By default, we use Adam with `lr=0.01`.
- **loss_fn** (*callable*) – A loss function which takes inputs are `gpmodule.model`, `gpmodule.guide`, and returns ELBO loss. By default, `loss_fn=TraceMeanField_ELBO().differentiable_loss`.
- **retain_graph** (*bool*) – An optional flag of `torch.autograd.backward`.
- **num_steps** (*int*) – Number of steps to run SVI.

Returns a list of losses during the training procedure

Return type list

CHAPTER 19

Minipyro

19.1 Mini Pyro

This file contains a minimal implementation of the Pyro Probabilistic Programming Language. The API (method signatures, etc.) match that of the full implementation as closely as possible. This file is independent of the rest of Pyro, with the exception of the `pyro.distributions` module.

An accompanying example that makes use of this implementation can be found at examples/minipyro.py.

class Adam(*optim_args*)
Bases: `object`

__call__(*params*)

class JitTrace_ELBO(***kwargs*)
Bases: `object`

__call__(*model*, *guide*, **args*)

class Messenger(*fn=None*)
Bases: `object`

__call__(**args*, ***kwargs*)

postprocess_message(*msg*)

process_message(*msg*)

class PlateMessenger(*fn*, *size*, *dim*)
Bases: *pyro.contrib.minipyro.Messenger*

process_message(*msg*)

class SVI(*model*, *guide*, *optim*, *loss*)
Bases: `object`

step(**args*, ***kwargs*)

Trace_ELBO(***kwargs*)

apply_stack(*msg*)

class block(*fn=None*, *hide_fn=<function block.<lambda>>*)
Bases: *pyro.contrib.minipyro.Messenger*

process_message(*msg*)

elbo(*model*, *guide*, **args*, ***kwargs*)

get_param_store()

param(*name*, *init_value=None*, *constraint=Real()*, *event_dim=None*)

plate(*name*, *size*, *dim=None*)

class replay(*fn*, *guide_trace*)
Bases: *pyro.contrib.minipyro.Messenger*

process_message(*msg*)

sample(*name*, *fn*, **args*, ***kwargs*)

class seed(*fn=None*, *rng_seed=None*)
Bases: *pyro.contrib.minipyro.Messenger*

class trace(*fn=None*)
Bases: *pyro.contrib.minipyro.Messenger*

get_trace(**args*, ***kwargs*)

postprocess_message(*msg*)

CHAPTER 20

Optimal Experiment Design

Tasks such as choosing the next question to ask in a psychology study, designing an election polling strategy, and deciding which compounds to synthesize and test in biological sciences are all fundamentally asking the same question: how do we design an experiment to maximize the information gathered? Pyro is designed to support automated optimal experiment design: specifying a model and guide is enough to obtain optimal designs for many different kinds of experiment scenarios. Check out our experimental design tutorials that use Pyro to design an adaptive psychology study that uses past data to select the next question, and design an election polling strategy that aims to give the strongest prediction about the eventual winner of the election.

Bayesian optimal experimental design (BOED) is a powerful methodology for tackling experimental design problems and is the framework adopted by Pyro. In the BOED framework, we begin with a Bayesian model with a likelihood $p(y|\theta, d)$ and a prior $p(\theta)$ on the target latent variables. In Pyro, any fully Bayesian model can be used in the BOED framework. The sample sites corresponding to experimental outcomes are the *observation* sites, those corresponding to latent variables of interest are the *target* sites. The design d is the argument to the model, and is not a random variable.

In the BOED framework, we choose the design that optimizes the expected information gain (EIG) on the targets θ from running the experiment

$$\text{EIG}(d) = \mathbf{E}_{p(y|d)}[H[p(\theta)]H[p(\theta|y, d)]] \,,$$

where $H[]$ represents the entropy and $p(\theta|y, d) \propto p(\theta)p(y|\theta, d)$ is the posterior we get from running the experiment with design d and observing y. In other words, the optimal design is the one that, in expectation over possible future observations, most reduces posterior entropy over the target latent variables. If the predictive model is correct, this forms a design strategy that is (one-step) optimal from an information-theoretic viewpoint. For further details, see [1, 2].

The *pyro.contrib.oed* module provides tools to create optimal experimental designs for Pyro models. In particular, it provides estimators for the expected information gain (EIG).

To estimate the EIG for a particular design, we first set up our Pyro model. For example:

```
def model(design):

    # This line allows batching of designs, treating all batch dimensions as␣
↪independent
```

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```
    with pyro.plate_stack("plate_stack", design.shape):

        # We use a Normal prior for theta
        theta = pyro.sample("theta", dist.Normal(torch.tensor(0.0), torch.tensor(1.
↪0)))

        # We use a simple logistic regression model for the likelihood
        logit_p = theta - design
        y = pyro.sample("y", dist.Bernoulli(logits=logit_p))

        return y
```

We then select an appropriate EIG estimator, such as:

```
eig = nmc_eig(model, design, observation_labels=["y"], target_labels=["theta"],␣
↪N=2500, M=50)
```

It is possible to estimate the EIG across a grid of designs:

```
designs = torch.stack([design1, design2], dim=0)
```

to find the best design from a number of options.

[1] Chaloner, Kathryn, and Isabella Verdinelli. "Bayesian experimental design: A review." Statistical Science (1995): 273-304.

[2] Foster, Adam, et al. "Variational Bayesian Optimal Experimental Design." arXiv preprint arXiv:1903.05480 (2019).

20.1 Expected Information Gain

laplace_eig(*model*, *design*, *observation_labels*, *target_labels*, *guide*, *loss*, *optim*, *num_steps*, *final_num_samples*, *y_dist=None*, *eig=True*, ***prior_entropy_kwargs*)

Estimates the expected information gain (EIG) by making repeated Laplace approximations to the posterior.

Parameters

- **model** (*function*) – Pyro stochastic function taking *design* as only argument.
- **design** (*torch.Tensor*) – Tensor of possible designs.
- **observation_labels** (*list*) – labels of sample sites to be regarded as observables.
- **target_labels** (*list*) – labels of sample sites to be regarded as latent variables of interest, i.e. the sites that we wish to gain information about.
- **guide** (*function*) – Pyro stochastic function corresponding to *model*.
- **loss** – a Pyro loss such as *pyro.infer.Trace_ELBO().differentiable_loss*.
- **optim** – optimizer for the loss
- **num_steps** (*int*) – Number of gradient steps to take per sampled pseudo-observation.
- **final_num_samples** (*int*) – Number of *y* samples (pseudo-observations) to take.
- **y_dist** – Distribution to sample *y* from- if *None* we use the Bayesian marginal distribution.

- **eig** (*bool*) – Whether to compute the EIG or the average posterior entropy (APE). The EIG is given by *EIG = prior entropy - APE*. If *True*, the prior entropy will be estimated analytically, or by Monte Carlo as appropriate for the *model*. If *False* the APE is returned.
- **prior_entropy_kwargs** (*dict*) – parameters for estimating the prior entropy: *num_prior_samples* indicating the number of samples for a MC estimate of prior entropy, and *mean_field* indicating if an analytic form for a mean-field prior should be tried.

Returns EIG estimate, optionally includes full optimization history

Return type torch.Tensor

vi_eig(*model*, *design*, *observation_labels*, *target_labels*, *vi_parameters*, *is_parameters*, *y_dist=None*, *eig=True*, ***prior_entropy_kwargs*)

Deprecated since version 0.4.1: Use *posterior_eig* instead.

Estimates the expected information gain (EIG) using variational inference (VI).

The APE is defined as

$$APE(d) = E_{Y\sim p(y|\theta,d)}[H(p(\theta|Y,d))]$$

where $H[p(x)]$ is the differential entropy. The APE is related to expected information gain (EIG) by the equation

$$EIG(d) = H[p(\theta)] - APE(d)$$

in particular, minimising the APE is equivalent to maximising EIG.

Parameters

- **model** (*function*) – A pyro model accepting *design* as only argument.
- **design** (*torch.Tensor*) – Tensor representation of design
- **observation_labels** (*list*) – A subset of the sample sites present in *model*. These sites are regarded as future observations and other sites are regarded as latent variables over which a posterior is to be inferred.
- **target_labels** (*list*) – A subset of the sample sites over which the posterior entropy is to be measured.
- **vi_parameters** (*dict*) – Variational inference parameters which should include: *optim*: an instance of `pyro.Optim`, *guide*: a guide function compatible with *model*, *num_steps*: the number of VI steps to make, and *loss*: the loss function to use for VI
- **is_parameters** (*dict*) – Importance sampling parameters for the marginal distribution of Y. May include *num_samples*: the number of samples to draw from the marginal.
- **y_dist** (*pyro.distributions.Distribution*) – (optional) the distribution assumed for the response variable Y
- **eig** (*bool*) – Whether to compute the EIG or the average posterior entropy (APE). The EIG is given by *EIG = prior entropy - APE*. If *True*, the prior entropy will be estimated analytically, or by Monte Carlo as appropriate for the *model*. If *False* the APE is returned.
- **prior_entropy_kwargs** (*dict*) – parameters for estimating the prior entropy: *num_prior_samples* indicating the number of samples for a MC estimate of prior entropy, and *mean_field* indicating if an analytic form for a mean-field prior should be tried.

Returns EIG estimate, optionally includes full optimization history

Return type torch.Tensor

nmc_eig(*model*, *design*, *observation_labels*, *target_labels=None*, *N=100*, *M=10*, *M_prime=None*, *independent_priors=False*)

Nested Monte Carlo estimate of the expected information gain (EIG). The estimate is, when there are not any random effects,

$$\frac{1}{N}\sum_{n=1}^{N}\log p(y_n|\theta_n,d)-\frac{1}{N}\sum_{n=1}^{N}\log\left(\frac{1}{M}\sum_{m=1}^{M}p(y_n|\theta_m,d)\right)$$

where $\theta_n, y_n \sim p(\theta, y|d)$ and $\theta_m \sim p(\theta)$. The estimate in the presence of random effects is

$$\frac{1}{N}\sum_{n=1}^{N}\log\left(\frac{1}{M'}\sum_{m=1}^{M'}p(y_n|\theta_n,\widetilde{\theta}_{nm},d)\right)-\frac{1}{N}\sum_{n=1}^{N}\log\left(\frac{1}{M}\sum_{m=1}^{M}p(y_n|\theta_m,\widetilde{\theta}_m,d)\right)$$

where $\widetilde{\theta}$ are the random effects with $\widetilde{\theta}_{nm} \sim p(\widetilde{\theta}|\theta=\theta_n)$ and $\theta_m, \widetilde{\theta}_m \sim p(\theta, \widetilde{\theta})$. The latter form is used when *M_prime != None*.

Parameters

- **model** (*function*) – A pyro model accepting *design* as only argument.
- **design** (*torch.Tensor*) – Tensor representation of design
- **observation_labels** (*list*) – A subset of the sample sites present in *model*. These sites are regarded as future observations and other sites are regarded as latent variables over which a posterior is to be inferred.
- **target_labels** (*list*) – A subset of the sample sites over which the posterior entropy is to be measured.
- **N** (*int*) – Number of outer expectation samples.
- **M** (*int*) – Number of inner expectation samples for *p(y|d)*.
- **M_prime** (*int*) – Number of samples for *p(y | theta, d)* if required.
- **independent_priors** (*bool*) – Only used when *M_prime* is not *None*. Indicates whether the prior distributions for the target variables and the nuisance variables are independent. In this case, it is not necessary to sample the targets conditional on the nuisance variables.

Returns EIG estimate, optionally includes full optimization history

Return type torch.Tensor

donsker_varadhan_eig(*model*, *design*, *observation_labels*, *target_labels*, *num_samples*, *num_steps*, *T*, *optim*, *return_history=False*, *final_design=None*, *final_num_samples=None*)

Donsker-Varadhan estimate of the expected information gain (EIG).

The Donsker-Varadhan representation of EIG is

$$\sup_{T} E_{p(y,\theta|d)}[T(y,\theta)]-\log E_{p(y|d)p(\theta)}[\exp(T(\bar{y},\bar{\theta}))]$$

where T is any (measurable) function.

This methods optimises the loss function over a pre-specified class of functions *T*.

Parameters

- **model** (*function*) – A pyro model accepting *design* as only argument.
- **design** (*torch.Tensor*) – Tensor representation of design

- **observation_labels** (*list*) – A subset of the sample sites present in *model*. These sites are regarded as future observations and other sites are regarded as latent variables over which a posterior is to be inferred.
- **target_labels** (*list*) – A subset of the sample sites over which the posterior entropy is to be measured.
- **num_samples** (*int*) – Number of samples per iteration.
- **num_steps** (*int*) – Number of optimization steps.
- **or torch.nn.Module T** (*function*) – optimisable function T for use in the Donsker-Varadhan loss function.
- **optim** (*pyro.optim.Optim*) – Optimiser to use.
- **return_history** (*bool*) – If *True*, also returns a tensor giving the loss function at each step of the optimization.
- **final_design** (*torch.Tensor*) – The final design tensor to evaluate at. If *None*, uses *design*.
- **final_num_samples** (*int*) – The number of samples to use at the final evaluation, If *None, uses 'num_samples*.

Returns EIG estimate, optionally includes full optimization history

Return type torch.Tensor or tuple

posterior_eig(*model*, *design*, *observation_labels*, *target_labels*, *num_samples*, *num_steps*, *guide*, *optim*, *return_history=False*, *final_design=None*, *final_num_samples=None*, *eig=True*, *prior_entropy_kwargs={}*, **args*, ***kwargs*)

Posterior estimate of expected information gain (EIG) computed from the average posterior entropy (APE) using $EIG(d) = H[p(\theta)] - APE(d)$. See [1] for full details.

The posterior representation of APE is

$\sup_q \ E_{p(y,\theta|d)}[\log q(\theta|y,d)]$

where q is any distribution on θ.

This method optimises the loss over a given *guide* family representing q.

[1] Foster, Adam, et al. "Variational Bayesian Optimal Experimental Design." arXiv preprint arXiv:1903.05480 (2019).

Parameters

- **model** (*function*) – A pyro model accepting *design* as only argument.
- **design** (*torch.Tensor*) – Tensor representation of design
- **observation_labels** (*list*) – A subset of the sample sites present in *model*. These sites are regarded as future observations and other sites are regarded as latent variables over which a posterior is to be inferred.
- **target_labels** (*list*) – A subset of the sample sites over which the posterior entropy is to be measured.
- **num_samples** (*int*) – Number of samples per iteration.
- **num_steps** (*int*) – Number of optimization steps.
- **guide** (*function*) – guide family for use in the (implicit) posterior estimation. The parameters of *guide* are optimised to maximise the posterior objective.
- **optim** (*pyro.optim.Optim*) – Optimiser to use.

- **return_history** (*bool*) – If *True*, also returns a tensor giving the loss function at each step of the optimization.
- **final_design** (*torch.Tensor*) – The final design tensor to evaluate at. If *None*, uses *design*.
- **final_num_samples** (*int*) – The number of samples to use at the final evaluation, If *None, uses 'num_samples*.
- **eig** (*bool*) – Whether to compute the EIG or the average posterior entropy (APE). The EIG is given by *EIG = prior entropy - APE*. If *True*, the prior entropy will be estimated analytically, or by Monte Carlo as appropriate for the *model*. If *False* the APE is returned.
- **prior_entropy_kwargs** (*dict*) – parameters for estimating the prior entropy: *num_prior_samples* indicating the number of samples for a MC estimate of prior entropy, and *mean_field* indicating if an analytic form for a mean-field prior should be tried.

Returns EIG estimate, optionally includes full optimization history

Return type torch.Tensor or tuple

marginal_eig(*model*, *design*, *observation_labels*, *target_labels*, *num_samples*, *num_steps*, *guide*, *optim*, *return_history=False*, *final_design=None*, *final_num_samples=None*)

Estimate EIG by estimating the marginal entropy $p(y|d)$. See [1] for full details.

The marginal representation of EIG is

$$\inf_q \; E_{p(y,\theta|d)}\left[\log \frac{p(y|\theta,d)}{q(y|d)}\right]$$

where q is any distribution on y. A variational family for q is specified in the *guide*.

Warning: This method does **not** estimate the correct quantity in the presence of random effects.

[1] Foster, Adam, et al. "Variational Bayesian Optimal Experimental Design." arXiv preprint arXiv:1903.05480 (2019).

Parameters

- **model** (*function*) – A pyro model accepting *design* as only argument.
- **design** (*torch.Tensor*) – Tensor representation of design
- **observation_labels** (*list*) – A subset of the sample sites present in *model*. These sites are regarded as future observations and other sites are regarded as latent variables over which a posterior is to be inferred.
- **target_labels** (*list*) – A subset of the sample sites over which the posterior entropy is to be measured.
- **num_samples** (*int*) – Number of samples per iteration.
- **num_steps** (*int*) – Number of optimization steps.
- **guide** (*function*) – guide family for use in the marginal estimation. The parameters of *guide* are optimised to maximise the log-likelihood objective.
- **optim** (*pyro.optim.Optim*) – Optimiser to use.
- **return_history** (*bool*) – If *True*, also returns a tensor giving the loss function at each step of the optimization.
- **final_design** (*torch.Tensor*) – The final design tensor to evaluate at. If *None*, uses *design*.

- **final_num_samples** (*int*) – The number of samples to use at the final evaluation, If *None, uses 'num_samples*.

Returns EIG estimate, optionally includes full optimization history

Return type torch.Tensor or tuple

lfire_eig(*model*, *design*, *observation_labels*, *target_labels*, *num_y_samples*, *num_theta_samples*, *num_steps*, *classifier*, *optim*, *return_history=False*, *final_design=None*, *final_num_samples=None*)

Estimates the EIG using the method of Likelihood-Free Inference by Ratio Estimation (LFIRE) as in [1]. LFIRE is run separately for several samples of θ.

[1] Kleinegesse, Steven, and Michael Gutmann. "Efficient Bayesian Experimental Design for Implicit Models." arXiv preprint arXiv:1810.09912 (2018).

Parameters

- **model** (*function*) – A pyro model accepting *design* as only argument.
- **design** (*torch.Tensor*) – Tensor representation of design
- **observation_labels** (*list*) – A subset of the sample sites present in *model*. These sites are regarded as future observations and other sites are regarded as latent variables over which a posterior is to be inferred.
- **target_labels** (*list*) – A subset of the sample sites over which the posterior entropy is to be measured.
- **num_y_samples** (*int*) – Number of samples to take in y for each θ.
- **num_steps** (*int*) – Number of optimization steps.
- **classifier** (*function*) – a Pytorch or Pyro classifier used to distinguish between samples of y under $p(y|d)$ and samples under $p(y|\theta, d)$ for some θ.
- **optim** (*pyro.optim.Optim*) – Optimiser to use.
- **return_history** (*bool*) – If *True*, also returns a tensor giving the loss function at each step of the optimization.
- **final_design** (*torch.Tensor*) – The final design tensor to evaluate at. If *None*, uses *design*.
- **final_num_samples** (*int*) – The number of samples to use at the final evaluation, If *None, uses 'num_samples*.

Param int num_theta_samples: Number of initial samples in θ to take. The likelihood ratio is estimated by LFIRE for each sample.

Returns EIG estimate, optionally includes full optimization history

Return type torch.Tensor or tuple

vnmc_eig(*model*, *design*, *observation_labels*, *target_labels*, *num_samples*, *num_steps*, *guide*, *optim*, *return_history=False*, *final_design=None*, *final_num_samples=None*)

Estimates the EIG using Variational Nested Monte Carlo (VNMC). The VNMC estimate [1] is

$$\frac{1}{N}\sum_{n=1}^{N}\left[\log p(y_n|\theta_n,d) - \log\left(\frac{1}{M}\sum_{m=1}^{M}\frac{p(\theta_{mn})p(y_n|\theta_{mn},d)}{q(\theta_{mn}|y_n)}\right)\right]$$

where $q(\theta|y)$ is the learned variational posterior approximation and $\theta_n, y_n \sim p(\theta, y|d)$, $\theta_{mn} \sim q(\theta|y = y_n)$.

As $N \to \infty$ this is an upper bound on EIG. We minimise this upper bound by stochastic gradient descent.

Warning: This method cannot be used in the presence of random effects.

[1] Foster, Adam, et al. "Variational Bayesian Optimal Experimental Design." arXiv preprint arXiv:1903.05480 (2019).

Parameters

- **model** (*function*) – A pyro model accepting *design* as only argument.
- **design** (*torch.Tensor*) – Tensor representation of design
- **observation_labels** (*list*) – A subset of the sample sites present in *model*. These sites are regarded as future observations and other sites are regarded as latent variables over which a posterior is to be inferred.
- **target_labels** (*list*) – A subset of the sample sites over which the posterior entropy is to be measured.
- **num_samples** (*tuple*) – Number of (N, M) samples per iteration.
- **num_steps** (*int*) – Number of optimization steps.
- **guide** (*function*) – guide family for use in the posterior estimation. The parameters of *guide* are optimised to minimise the VNMC upper bound.
- **optim** (*pyro.optim.Optim*) – Optimiser to use.
- **return_history** (*bool*) – If *True*, also returns a tensor giving the loss function at each step of the optimization.
- **final_design** (*torch.Tensor*) – The final design tensor to evaluate at. If *None*, uses *design*.
- **final_num_samples** (*tuple*) – The number of (N, M) samples to use at the final evaluation, If *None, uses 'num_samples*.

Returns EIG estimate, optionally includes full optimization history

Return type torch.Tensor or tuple

20.2 Generalised Linear Mixed Models

Warning: This module will eventually be deprecated in favor of brmp

The *pyro.contrib.oed.glmm* module provides models and guides for generalised linear mixed models (GLMM). It also includes the Normal-inverse-gamma family.

To create a classical Bayesian linear model, use:

```
from pyro.contrib.oed.glmm import known_covariance_linear_model

# Note: coef is a p-vector, observation_sd is a scalar
# Here, p=1 (one feature)
model = known_covariance_linear_model(coef_mean=torch.tensor([0.]),
                                      coef_sd=torch.tensor([10.]),
                                      observation_sd=torch.tensor(2.))
```

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```
# An n x p design tensor
# Here, n=2 (two observations)
design = torch.tensor(torch.tensor([[1.], [-1.]]))

model(design)
```

A non-linear link function may be introduced, for instance:

```
from pyro.contrib.oed.glmm import logistic_regression_model

# No observation_sd is needed for logistic models
model = logistic_regression_model(coef_mean=torch.tensor([0.]),
                                  coef_sd=torch.tensor([10.]))
```

Random effects may be incorporated as regular Bayesian regression coefficients. For random effects with a shared covariance matrix, see `pyro.contrib.oed.glmm.lmer_model()`.

CHAPTER 21

Random Variables

21.1 Random Variable

class RandomVariable(*distribution*)

Bases: pyro.contrib.randomvariable.random_variable.RVMagicOps, pyro.contrib.randomvariable.random_variable.RVChainOps

EXPERIMENTAL random variable container class around a distribution

Representation of a distribution interpreted as a random variable. Rather than directly manipulating a probability density by applying pointwise transformations to it, this allows for simple arithmetic transformations of the random variable the distribution represents. For more flexibility, consider using the *transform* method. Note that if you perform a non-invertible transform (like *abs(X)* or *X**2), certain things might not work properly.

Can switch between *RandomVariable* and *Distribution* objects with the convenient *Distribution.rv* and *RandomVariable.dist* properties.

Supports either chaining operations or arithmetic operator overloading.

Example usage:

```
# This should be equivalent to an Exponential distribution.
RandomVariable(Uniform(0, 1)).log().neg().dist

# These two distributions Y1, Y2 should be the same
X = Uniform(0, 1).rv
Y1 = X.mul(4).pow(0.5).sub(1).abs().neg().dist
Y2 = (-abs((4*X)**(0.5) - 1)).dist
```

dist

Convenience property for exposing the distribution underlying the random variable.

Returns The *Distribution* object underlying the random variable

Return type Distribution

transform(*t: torch.distributions.transforms.Transform*)

Performs a transformation on the distribution underlying the RV.

Parameters **t** (*Transform*) – The transformation (or sequence of transformations) to be applied to the distribution. There are many examples to be found in *torch.distributions.transforms* and *pyro.distributions.transforms*, or you can subclass directly from *Transform*.

Returns The transformed *RandomVariable*

Return type *RandomVariable*

CHAPTER 22

Time Series

The *pyro.contrib.timeseries* module provides a collection of Bayesian time series models useful for forecasting applications.

See the GP example for example usage.

22.1 Abstract Models

class TimeSeriesModel(*name=''*)

Bases: *pyro.nn.module.PyroModule*

Base class for univariate and multivariate time series models.

log_prob(*targets*)

Log probability function.

Parameters **targets** (*torch.Tensor*) – A 2-dimensional tensor of real-valued targets of shape `(T, obs_dim)`, where `T` is the length of the time series and `obs_dim` is the dimension of the real-valued `targets` at each time step

Returns torch.Tensor A 0-dimensional log probability for the case of properly multivariate time series models in which the output dimensions are correlated; otherwise returns a 1-dimensional tensor of log probabilities for batched univariate time series models.

forecast(*targets*, *dts*)

Parameters

- **targets** (*torch.Tensor*) – A 2-dimensional tensor of real-valued targets of shape `(T, obs_dim)`, where `T` is the length of the time series and `obs_dim` is the dimension of the real-valued targets at each time step. These represent the training data that are conditioned on for the purpose of making forecasts.
- **dts** (*torch.Tensor*) – A 1-dimensional tensor of times to forecast into the future, with zero corresponding to the time of the final target `targets[-1]`.

Returns torch.distributions.Distribution Returns a predictive distribution with batch shape `(S,)` and event shape `(obs_dim,)`, where `S` is the size of `dts`. That is, the resulting predictive distributions do not encode correlations between distinct times in `dts`.

get_dist()
Get a *Distribution* object corresponding to this time series model. Often this is a *GaussianHMM*.

22.2 Gaussian Processes

class IndependentMaternGP(*nu=1.5*, *dt=1.0*, *obs_dim=1*, *length_scale_init=None*, *kernel_scale_init=None*, *obs_noise_scale_init=None*)
Bases: *pyro.contrib.timeseries.base.TimeSeriesModel*

A time series model in which each output dimension is modeled independently with a univariate Gaussian Process with a Matern kernel. The targets are assumed to be evenly spaced in time. Training and inference are logarithmic in the length of the time series T.

Parameters

- **nu** (*float*) – The order of the Matern kernel; one of 0.5, 1.5 or 2.5.
- **dt** (*float*) – The time spacing between neighboring observations of the time series.
- **obs_dim** (*int*) – The dimension of the targets at each time step.
- **length_scale_init** (*torch.Tensor*) – optional initial values for the kernel length scale given as a `obs_dim`-dimensional tensor
- **kernel_scale_init** (*torch.Tensor*) – optional initial values for the kernel scale given as a `obs_dim`-dimensional tensor
- **obs_noise_scale_init** (*torch.Tensor*) – optional initial values for the observation noise scale given as a `obs_dim`-dimensional tensor

get_dist(*duration=None*)
Get the *GaussianHMM* distribution that corresponds to `obs_dim`-many independent Matern GPs.

Parameters **duration** (*int*) – Optional size of the time axis `event_shape[0]`. This is required when sampling from homogeneous HMMs whose parameters are not expanded along the time axis.

log_prob(*targets*)

Parameters **targets** (*torch.Tensor*) – A 2-dimensional tensor of real-valued targets of shape `(T, obs_dim)`, where `T` is the length of the time series and `obs_dim` is the dimension of the real-valued `targets` at each time step

Returns torch.Tensor A 1-dimensional tensor of log probabilities of shape `(obs_dim,)`

forecast(*targets*, *dts*)

Parameters

- **targets** (*torch.Tensor*) – A 2-dimensional tensor of real-valued targets of shape `(T, obs_dim)`, where `T` is the length of the time series and `obs_dim` is the dimension of the real-valued targets at each time step. These represent the training data that are conditioned on for the purpose of making forecasts.
- **dts** (*torch.Tensor*) – A 1-dimensional tensor of times to forecast into the future, with zero corresponding to the time of the final target `targets[-1]`.

Returns torch.distributions.Normal Returns a predictive Normal distribution with batch shape `(S,)` and event shape `(obs_dim,)`, where `S` is the size of `dts`.

class LinearlyCoupledMaternGP(*nu=1.5*, *dt=1.0*, *obs_dim=2*, *num_gps=1*, *length_scale_init=None*, *kernel_scale_init=None*, *obs_noise_scale_init=None*)

Bases: *pyro.contrib.timeseries.base.TimeSeriesModel*

A time series model in which each output dimension is modeled as a linear combination of shared univariate Gaussian Processes with Matern kernels.

In more detail, the generative process is:

$y_i(t) = \sum_j A_{ij} f_j(t) + \epsilon_i(t)$

The targets y_i are assumed to be evenly spaced in time. Training and inference are logarithmic in the length of the time series T.

Parameters

- **nu** (*float*) – The order of the Matern kernel; one of 0.5, 1.5 or 2.5.
- **dt** (*float*) – The time spacing between neighboring observations of the time series.
- **obs_dim** (*int*) – The dimension of the targets at each time step.
- **num_gps** (*int*) – The number of independent GPs that are mixed to model the time series. Typical values might be $_{\text{gp}} \in [_{\text{obs}}/2, _{\text{obs}}]$
- **length_scale_init** (*torch.Tensor*) – optional initial values for the kernel length scale given as a `num_gps`-dimensional tensor
- **kernel_scale_init** (*torch.Tensor*) – optional initial values for the kernel scale given as a `num_gps`-dimensional tensor
- **obs_noise_scale_init** (*torch.Tensor*) – optional initial values for the observation noise scale given as a `obs_dim`-dimensional tensor

get_dist(*duration=None*)

Get the *GaussianHMM* distribution that corresponds to a *LinearlyCoupledMaternGP*.

Parameters **duration** (*int*) – Optional size of the time axis `event_shape[0]`. This is required when sampling from homogeneous HMMs whose parameters are not expanded along the time axis.

log_prob(*targets*)

Parameters **targets** (*torch.Tensor*) – A 2-dimensional tensor of real-valued targets of shape `(T, obs_dim)`, where `T` is the length of the time series and `obs_dim` is the dimension of the real-valued `targets` at each time step

Returns torch.Tensor a (scalar) log probability

forecast(*targets*, *dts*)

Parameters

- **targets** (*torch.Tensor*) – A 2-dimensional tensor of real-valued targets of shape `(T, obs_dim)`, where `T` is the length of the time series and `obs_dim` is the dimension of the real-valued targets at each time step. These represent the training data that are conditioned on for the purpose of making forecasts.
- **dts** (*torch.Tensor*) – A 1-dimensional tensor of times to forecast into the future, with zero corresponding to the time of the final target `targets[-1]`.

Returns torch.distributions.MultivariateNormal Returns a predictive MultivariateNormal distribution with batch shape `(S,)` and event shape `(obs_dim,)`, where `S` is the size of `dts`.

class DependentMaternGP(*nu=1.5*, *dt=1.0*, *obs_dim=1*, *linearly_coupled=False*, *length_scale_init=None*, *obs_noise_scale_init=None*)

Bases: *pyro.contrib.timeseries.base.TimeSeriesModel*

A time series model in which each output dimension is modeled as a univariate Gaussian Process with a Matern kernel. The different output dimensions become correlated because the Gaussian Processes are driven by a correlated Wiener process; see reference [1] for details. If, in addition, *linearly_coupled* is True, additional correlation is achieved through linear mixing as in *LinearlyCoupledMaternGP*. The targets are assumed to be evenly spaced in time. Training and inference are logarithmic in the length of the time series T.

Parameters

- **nu** (*float*) – The order of the Matern kernel; must be 1.5.
- **dt** (*float*) – The time spacing between neighboring observations of the time series.
- **obs_dim** (*int*) – The dimension of the targets at each time step.
- **linearly_coupled** (*bool*) – Whether to linearly mix the various gaussian processes in the likelihood. Defaults to False.
- **length_scale_init** (*torch.Tensor*) – optional initial values for the kernel length scale given as a `obs_dim`-dimensional tensor
- **obs_noise_scale_init** (*torch.Tensor*) – optional initial values for the observation noise scale given as a `obs_dim`-dimensional tensor

References [1] "Dependent Matern Processes for Multivariate Time Series," Alexander Vandenberg-Rodes, Babak Shahbaba.

get_dist(*duration=None*)

Get the *GaussianHMM* distribution that corresponds to a *DependentMaternGP*

Parameters **duration** (*int*) – Optional size of the time axis `event_shape[0]`. This is required when sampling from homogeneous HMMs whose parameters are not expanded along the time axis.

log_prob(*targets*)

Parameters **targets** (*torch.Tensor*) – A 2-dimensional tensor of real-valued targets of shape `(T, obs_dim)`, where `T` is the length of the time series and `obs_dim` is the dimension of the real-valued `targets` at each time step

Returns torch.Tensor A (scalar) log probability

forecast(*targets*, *dts*)

Parameters

- **targets** (*torch.Tensor*) – A 2-dimensional tensor of real-valued targets of shape `(T, obs_dim)`, where `T` is the length of the time series and `obs_dim` is the dimension of the real-valued targets at each time step. These represent the training data that are conditioned on for the purpose of making forecasts.
- **dts** (*torch.Tensor*) – A 1-dimensional tensor of times to forecast into the future, with zero corresponding to the time of the final target `targets[-1]`.

Returns torch.distributions.MultivariateNormal Returns a predictive MultivariateNormal distribution with batch shape `(S,)` and event shape `(obs_dim,)`, where `S` is the size of `dts`.

22.3 Linear Gaussian State Space Models

class GenericLGSSM(*obs_dim=1*, *state_dim=2*, *obs_noise_scale_init=None*, *learnable_observation_loc=False*)

Bases: *pyro.contrib.timeseries.base.TimeSeriesModel*

A generic Linear Gaussian State Space Model parameterized with arbitrary time invariant transition and observation dynamics. The targets are (implicitly) assumed to be evenly spaced in time. Training and inference are logarithmic in the length of the time series T.

Parameters

- **obs_dim** (*int*) – The dimension of the targets at each time step.
- **state_dim** (*int*) – The dimension of latent state at each time step.
- **learnable_observation_loc** (*bool*) – whether the mean of the observation model should be learned or not; defaults to False.

get_dist(*duration=None*)

Get the *GaussianHMM* distribution that corresponds to *GenericLGSSM*.

Parameters **duration** (*int*) – Optional size of the time axis `event_shape[0]`. This is required when sampling from homogeneous HMMs whose parameters are not expanded along the time axis.

log_prob(*targets*)

Parameters **targets** (*torch.Tensor*) – A 2-dimensional tensor of real-valued targets of shape `(T, obs_dim)`, where `T` is the length of the time series and `obs_dim` is the dimension of the real-valued `targets` at each time step

Returns torch.Tensor A (scalar) log probability.

forecast(*targets*, *N_timesteps*)

Parameters

- **targets** (*torch.Tensor*) – A 2-dimensional tensor of real-valued targets of shape `(T, obs_dim)`, where `T` is the length of the time series and `obs_dim` is the dimension of the real-valued targets at each time step. These represent the training data that are conditioned on for the purpose of making forecasts.
- **N_timesteps** (*int*) – The number of timesteps to forecast into the future from the final target `targets[-1]`.

Returns torch.distributions.MultivariateNormal Returns a predictive MultivariateNormal distribution with batch shape `(N_timesteps,)` and event shape `(obs_dim,)`

class GenericLGSSMWithGPNoiseModel(*obs_dim=1*, *state_dim=2*, *nu=1.5*, *obs_noise_scale_init=None*, *length_scale_init=None*, *kernel_scale_init=None*, *learnable_observation_loc=False*)

Bases: *pyro.contrib.timeseries.base.TimeSeriesModel*

A generic Linear Gaussian State Space Model parameterized with arbitrary time invariant transition and observation dynamics together with separate Gaussian Process noise models for each output dimension. In more detail, the generative process is:

$$y_i(t) = \sum_j A_{ij} z_j(t) + f_i(t) + \epsilon_i(t)$$

where the latent variables $\mathbf{z}(t)$ follow generic time invariant Linear Gaussian dynamics and the $f_i(t)$ are Gaussian Processes with Matern kernels.

The targets are (implicitly) assumed to be evenly spaced in time. In particular a timestep of $dt = 1.0$ for the continuous-time GP dynamics corresponds to a single discrete step of the **z**-space dynamics. Training and inference are logarithmic in the length of the time series T.

Parameters

- **obs_dim** (*int*) – The dimension of the targets at each time step.
- **state_dim** (*int*) – The dimension of the **z** latent state at each time step.
- **nu** (*float*) – The order of the Matern kernel; one of 0.5, 1.5 or 2.5.
- **length_scale_init** (*torch.Tensor*) – optional initial values for the kernel length scale given as a `obs_dim`-dimensional tensor
- **kernel_scale_init** (*torch.Tensor*) – optional initial values for the kernel scale given as a `obs_dim`-dimensional tensor
- **obs_noise_scale_init** (*torch.Tensor*) – optional initial values for the observation noise scale given as a `obs_dim`-dimensional tensor
- **learnable_observation_loc** (*bool*) – whether the mean of the observation model should be learned or not; defaults to False.

get_dist(*duration=None*)

Get the *GaussianHMM* distribution that corresponds to *GenericLGSSMWithGPNoiseModel*.

Parameters **duration** (*int*) – Optional size of the time axis `event_shape[0]`. This is required when sampling from homogeneous HMMs whose parameters are not expanded along the time axis.

log_prob(*targets*)

Parameters **targets** (*torch.Tensor*) – A 2-dimensional tensor of real-valued targets of shape `(T, obs_dim)`, where `T` is the length of the time series and `obs_dim` is the dimension of the real-valued `targets` at each time step

Returns torch.Tensor A (scalar) log probability.

forecast(*targets*, *N_timesteps*)

Parameters

- **targets** (*torch.Tensor*) – A 2-dimensional tensor of real-valued targets of shape `(T, obs_dim)`, where `T` is the length of the time series and `obs_dim` is the dimension of the real-valued targets at each time step. These represent the training data that are conditioned on for the purpose of making forecasts.
- **N_timesteps** (*int*) – The number of timesteps to forecast into the future from the final target `targets[-1]`.

Returns torch.distributions.MultivariateNormal Returns a predictive MultivariateNormal distribution with batch shape `(N_timesteps,)` and event shape `(obs_dim,)`

CHAPTER 23

Tracking

23.1 Data Association

class MarginalAssignment(*exists_logits*, *assign_logits*, *bp_iters=None*)

Computes marginal data associations between objects and detections.

This assumes that each detection corresponds to zero or one object, and each object corresponds to zero or more detections. Specifically this does not assume detections have been partitioned into frames of mutual exclusion as is common in 2-D assignment problems.

Parameters

- **exists_logits** (*torch.Tensor*) – a tensor of shape `[num_objects]` representing per-object factors for existence of each potential object.
- **assign_logits** (*torch.Tensor*) – a tensor of shape `[num_detections, num_objects]` representing per-edge factors of assignment probability, where each edge denotes that a given detection associates with a single object.
- **bp_iters** (*int*) – optional number of belief propagation iterations. If unspecified or `None` an expensive exact algorithm will be used.

Variables

- **num_detections** (*int*) – the number of detections
- **num_objects** (*int*) – the number of (potentially existing) objects
- **exists_dist** (`pyro.distributions.Bernoulli`) – a mean field posterior distribution over object existence.
- **assign_dist** (`pyro.distributions.Categorical`) – a mean field posterior distribution over the object (or None) to which each detection associates. This has `.event_shape == (num_objects + 1,)` where the final element denotes spurious detection, and `.batch_shape == (num_frames, num_detections)`.

class MarginalAssignmentSparse(*num_objects*, *num_detections*, *edges*, *exists_logits*, *assign_logits*, *bp_iters*)

A cheap sparse version of *MarginalAssignment*.

Parameters

- **num_detections** (*int*) – the number of detections
- **num_objects** (*int*) – the number of (potentially existing) objects
- **edges** (*torch.LongTensor*) – a `[2, num_edges]`-shaped tensor of (detection, object) index pairs specifying feasible associations.
- **exists_logits** (*torch.Tensor*) – a tensor of shape `[num_objects]` representing per-object factors for existence of each potential object.
- **assign_logits** (*torch.Tensor*) – a tensor of shape `[num_edges]` representing per-edge factors of assignment probability, where each edge denotes that a given detection associates with a single object.
- **bp_iters** (*int*) – optional number of belief propagation iterations. If unspecified or `None` an expensive exact algorithm will be used.

Variables

- **num_detections** (*int*) – the number of detections
- **num_objects** (*int*) – the number of (potentially existing) objects
- **exists_dist** (`pyro.distributions.Bernoulli`) – a mean field posterior distribution over object existence.
- **assign_dist** (`pyro.distributions.Categorical`) – a mean field posterior distribution over the object (or None) to which each detection associates. This has `.event_shape == (num_objects + 1,)` where the final element denotes spurious detection, and `.batch_shape == (num_frames, num_detections)`.

class MarginalAssignmentPersistent(*exists_logits*, *assign_logits*, *bp_iters=None*, *bp_momentum=0.5*)

This computes marginal distributions of a multi-frame multi-object data association problem with an unknown number of persistent objects.

The inputs are factors in a factor graph (existence probabilites for each potential object and assignment probabilities for each object-detection pair), and the outputs are marginal distributions of posterior existence probability of each potential object and posterior assignment probabilites of each object-detection pair.

This assumes a shared (maximum) number of detections per frame; to handle variable number of detections, simply set corresponding elements of `assign_logits` to `-float('inf')`.

Parameters

- **exists_logits** (*torch.Tensor*) – a tensor of shape `[num_objects]` representing per-object factors for existence of each potential object.
- **assign_logits** (*torch.Tensor*) – a tensor of shape `[num_frames, num_detections, num_objects]` representing per-edge factors of assignment probability, where each edge denotes that at a given time frame a given detection associates with a single object.
- **bp_iters** (*int*) – optional number of belief propagation iterations. If unspecified or `None` an expensive exact algorithm will be used.
- **bp_momentum** (*float*) – optional momentum to use for belief propagation. Should be in the interval `[0,1)`.

Variables

- **num_frames** (*int*) – the number of time frames
- **num_detections** (*int*) – the (maximum) number of detections per frame
- **num_objects** (*int*) – the number of (potentially existing) objects
- **exists_dist** (pyro.distributions.Bernoulli) – a mean field posterior distribution over object existence.
- **assign_dist** (pyro.distributions.Categorical) – a mean field posterior distribution over the object (or None) to which each detection associates. This has `.event_shape == (num_objects + 1,)` where the final element denotes spurious detection, and `.batch_shape == (num_frames, num_detections)`.

compute_marginals(*exists_logits*, *assign_logits*)

This implements exact inference of pairwise marginals via enumeration. This is very expensive and is only useful for testing.

See *MarginalAssignment* for args and problem description.

compute_marginals_bp(*exists_logits*, *assign_logits*, *bp_iters*)

This implements approximate inference of pairwise marginals via loopy belief propagation, adapting the approach of [1].

See *MarginalAssignment* for args and problem description.

[1] Jason L. Williams, Roslyn A. Lau (2014) Approximate evaluation of marginal association probabilities with belief propagation https://arxiv.org/abs/1209.6299

compute_marginals_sparse_bp(*num_objects*, *num_detections*, *edges*, *exists_logits*, *assign_logits*, *bp_iters*)

This implements approximate inference of pairwise marginals via loopy belief propagation, adapting the approach of [1].

See *MarginalAssignmentSparse* for args and problem description.

[1] Jason L. Williams, Roslyn A. Lau (2014) Approximate evaluation of marginal association probabilities with belief propagation https://arxiv.org/abs/1209.6299

compute_marginals_persistent(*exists_logits*, *assign_logits*)

This implements exact inference of pairwise marginals via enumeration. This is very expensive and is only useful for testing.

See *MarginalAssignmentPersistent* for args and problem description.

compute_marginals_persistent_bp(*exists_logits*, *assign_logits*, *bp_iters*, *bp_momentum=0.5*)

This implements approximate inference of pairwise marginals via loopy belief propagation, adapting the approach of [1], [2].

See *MarginalAssignmentPersistent* for args and problem description.

[1] Jason L. Williams, Roslyn A. Lau (2014) Approximate evaluation of marginal association probabilities with belief propagation https://arxiv.org/abs/1209.6299

[2] Ryan Turner, Steven Bottone, Bhargav Avasarala (2014) A Complete Variational Tracker https://papers.nips.cc/paper/5572-a-complete-variational-tracker.pdf

23.2 Distributions

class EKFDistribution(*x0*, *P0*, *dynamic_model*, *measurement_cov*, *time_steps=1*, *dt=1.0*, *validate_args=None*)

Distribution over EKF states. See *EKFState*. Currently only supports *log_prob*.

Parameters

- **x0** (*torch.Tensor*) – PV tensor (mean)
- **P0** (*torch.Tensor*) – covariance
- **dynamic_model** – *DynamicModel* object
- **measurement_cov** (*torch.Tensor*) – measurement covariance
- **time_steps** (*int*) – number time step
- **dt** (*torch.Tensor*) – time step

filter_states(*value*)

Returns the ekf states given measurements

Parameters **value** (*torch.Tensor*) – measurement means of shape *(time_steps, event_shape)*

log_prob(*value*)

Returns the joint log probability of the innovations of a tensor of measurements

Parameters **value** (*torch.Tensor*) – measurement means of shape *(time_steps, event_shape)*

23.3 Dynamic Models

class DynamicModel(*dimension*, *dimension_pv*, *num_process_noise_parameters=None*)

Dynamic model interface.

Parameters

- **dimension** – native state dimension.
- **dimension_pv** – PV state dimension.
- **num_process_noise_parameters** – process noise parameter space dimension. This for UKF applications. Can be left as `None` for EKF and most other filters.

dimension

Native state dimension access.

dimension_pv

PV state dimension access.

num_process_noise_parameters

Process noise parameters space dimension access.

forward(*x*, *dt*, *do_normalization=True*)

Integrate native state `x` over time interval `dt`.

Parameters

- **x** – current native state. If the DynamicModel is non-differentiable, be sure to handle the case of `x` being augmented with process noise parameters.

- **dt** – time interval to integrate over.
- **do_normalization** – whether to perform normalization on output, e.g., mod'ing angles into an interval.

Returns Native state x integrated dt into the future.

geodesic_difference(*x1*, *x0*)

Compute and return the geodesic difference between 2 native states. This is a generalization of the Euclidean operation `x1 - x0`.

Parameters

- **x1** – native state.
- **x0** – native state.

Returns Geodesic difference between native states `x1` and `x2`.

mean2pv(*x*)

Compute and return PV state from native state. Useful for combining state estimates of different types in IMM (Interacting Multiple Model) filtering.

Parameters **x** – native state estimate mean.

Returns PV state estimate mean.

cov2pv(*P*)

Compute and return PV covariance from native covariance. Useful for combining state estimates of different types in IMM (Interacting Multiple Model) filtering.

Parameters **P** – native state estimate covariance.

Returns PV state estimate covariance.

process_noise_cov(*dt=0.0*)

Compute and return process noise covariance (Q).

Parameters **dt** – time interval to integrate over.

Returns Read-only covariance (Q). For a DifferentiableDynamicModel, this is the covariance of the native state `x` resulting from stochastic integration (for use with EKF). Otherwise, it is the covariance directly of the process noise parameters (for use with UKF).

process_noise_dist(*dt=0.0*)

Return a distribution object of state displacement from the process noise distribution over a time interval.

Parameters **dt** – time interval that process noise accumulates over.

Returns `MultivariateNormal`.

class DifferentiableDynamicModel(*dimension*, *dimension_pv*, *num_process_noise_parameters=None*)

DynamicModel for which state transition Jacobians can be efficiently calculated, usu. analytically or by automatic differentiation.

jacobian(*dt*)

Compute and return native state transition Jacobian (F) over time interval `dt`.

Parameters **dt** – time interval to integrate over.

Returns Read-only Jacobian (F) of integration map (f).

class Ncp(*dimension*, *sv2*)

NCP (Nearly-Constant Position) dynamic model. May be subclassed, e.g., with CWNV (Continuous White Noise Velocity) or DWNV (Discrete White Noise Velocity).

Parameters

- **dimension** – native state dimension.
- **sv2** – variance of velocity. Usually chosen so that the standard deviation is roughly half of the max velocity one would ever expect to observe.

forward(*x*, *dt*, *do_normalization=True*)
Integrate native state x over time interval dt.

Parameters

- **x** – current native state. If the DynamicModel is non-differentiable, be sure to handle the case of x being augmented with process noise parameters.
- **dt** – time interval to integrate over. do_normalization: whether to perform normalization on output, e.g., mod'ing angles into an interval. Has no effect for this subclass.

Returns Native state x integrated dt into the future.

mean2pv(*x*)
Compute and return PV state from native state. Useful for combining state estimates of different types in IMM (Interacting Multiple Model) filtering.

Parameters **x** – native state estimate mean.

Returns PV state estimate mean.

cov2pv(*P*)
Compute and return PV covariance from native covariance. Useful for combining state estimates of different types in IMM (Interacting Multiple Model) filtering.

Parameters **P** – native state estimate covariance.

Returns PV state estimate covariance.

jacobian(*dt*)
Compute and return cached native state transition Jacobian (F) over time interval dt.

Parameters **dt** – time interval to integrate over.

Returns Read-only Jacobian (F) of integration map (f).

process_noise_cov(*dt=0.0*)
Compute and return cached process noise covariance (Q).

Parameters **dt** – time interval to integrate over.

Returns Read-only covariance (Q) of the native state x resulting from stochastic integration (for use with EKF).

class Ncv(*dimension*, *sa2*)
NCV (Nearly-Constant Velocity) dynamic model. May be subclassed, e.g., with CWNA (Continuous White Noise Acceleration) or DWNA (Discrete White Noise Acceleration).

Parameters

- **dimension** – native state dimension.
- **sa2** – variance of acceleration. Usually chosen so that the standard deviation is roughly half of the max acceleration one would ever expect to observe.

forward(*x*, *dt*, *do_normalization=True*)
Integrate native state x over time interval dt.

Parameters

- **x** – current native state. If the DynamicModel is non-differentiable, be sure to handle the case of x being augmented with process noise parameters.
- **dt** – time interval to integrate over.
- **do_normalization** – whether to perform normalization on output, e.g., mod'ing angles into an interval. Has no effect for this subclass.

Returns Native state x integrated dt into the future.

mean2pv(*x*)
Compute and return PV state from native state. Useful for combining state estimates of different types in IMM (Interacting Multiple Model) filtering.

Parameters **x** – native state estimate mean.

Returns PV state estimate mean.

cov2pv(*P*)
Compute and return PV covariance from native covariance. Useful for combining state estimates of different types in IMM (Interacting Multiple Model) filtering.

Parameters **P** – native state estimate covariance.

Returns PV state estimate covariance.

jacobian(*dt*)
Compute and return cached native state transition Jacobian (F) over time interval dt.

Parameters **dt** – time interval to integrate over.

Returns Read-only Jacobian (F) of integration map (f).

process_noise_cov(*dt=0.0*)
Compute and return cached process noise covariance (Q).

Parameters **dt** – time interval to integrate over.

Returns Read-only covariance (Q) of the native state x resulting from stochastic integration (for use with EKF).

class NcpContinuous(*dimension*, *sv2*)
NCP (Nearly-Constant Position) dynamic model with CWNV (Continuous White Noise Velocity).

References: "Estimation with Applications to Tracking and Navigation" by Y. Bar- Shalom et al, 2001, p.269.

Parameters

- **dimension** – native state dimension.
- **sv2** – variance of velocity. Usually chosen so that the standard deviation is roughly half of the max velocity one would ever expect to observe.

process_noise_cov(*dt=0.0*)
Compute and return cached process noise covariance (Q).

Parameters **dt** – time interval to integrate over.

Returns Read-only covariance (Q) of the native state x resulting from stochastic integration (for use with EKF).

class NcvContinuous(*dimension*, *sa2*)
NCV (Nearly-Constant Velocity) dynamic model with CWNA (Continuous White Noise Acceleration).

References: "Estimation with Applications to Tracking and Navigation" by Y. Bar- Shalom et al, 2001, p.269.

Parameters

- **dimension** – native state dimension.
- **sa2** – variance of acceleration. Usually chosen so that the standard deviation is roughly half of the max acceleration one would ever expect to observe.

process_noise_cov(*dt=0.0*)
Compute and return cached process noise covariance (Q).

Parameters **dt** – time interval to integrate over.

Returns Read-only covariance (Q) of the native state x resulting from stochastic integration (for use with EKF).

class NcpDiscrete(*dimension*, *sv2*)
NCP (Nearly-Constant Position) dynamic model with DWNV (Discrete White Noise Velocity).

Parameters

- **dimension** – native state dimension.
- **sv2** – variance of velocity. Usually chosen so that the standard deviation is roughly half of the max velocity one would ever expect to observe.

References: "Estimation with Applications to Tracking and Navigation" by Y. Bar- Shalom et al, 2001, p.273.

process_noise_cov(*dt=0.0*)
Compute and return cached process noise covariance (Q).

Parameters **dt** – time interval to integrate over.

Returns Read-only covariance (Q) of the native state *x* resulting from stochastic integration (for use with EKF).

class NcvDiscrete(*dimension*, *sa2*)
NCV (Nearly-Constant Velocity) dynamic model with DWNA (Discrete White Noise Acceleration).

Parameters

- **dimension** – native state dimension.
- **sa2** – variance of acceleration. Usually chosen so that the standard deviation is roughly half of the max acceleration one would ever expect to observe.

References: "Estimation with Applications to Tracking and Navigation" by Y. Bar- Shalom et al, 2001, p.273.

process_noise_cov(*dt=0.0*)
Compute and return cached process noise covariance (Q).

Parameters **dt** – time interval to integrate over.

Returns Read-only covariance (Q) of the native state *x* resulting from stochastic integration (for use with EKF). (Note that this Q, modulo numerical error, has rank *dimension/2*. So, it is only positive semi-definite.)

23.4 Extended Kalman Filter

class EKFState(*dynamic_model*, *mean*, *cov*, *time=None*, *frame_num=None*)
State-Centric EKF (Extended Kalman Filter) for use with either an NCP (Nearly-Constant Position) or NCV

(Nearly-Constant Velocity) target dynamic model. Stores a target dynamic model, state estimate, and state time. Incoming `Measurement` provide sensor information for updates.

Warning: For efficiency, the dynamic model is only shallow-copied. Make a deep copy outside as necessary to protect against unexpected changes.

Parameters

- **dynamic_model** – target dynamic model.
- **mean** – mean of target state estimate.
- **cov** – covariance of target state estimate.
- **time** – time of state estimate.

dynamic_model
Dynamic model access.

dimension
Native state dimension access.

mean
Native state estimate mean access.

cov
Native state estimate covariance access.

dimension_pv
PV state dimension access.

mean_pv
Compute and return cached PV state estimate mean.

cov_pv
Compute and return cached PV state estimate covariance.

time
Continuous State time access.

frame_num
Discrete State time access.

predict(*dt=None*, *destination_time=None*, *destination_frame_num=None*)
Use dynamic model to predict (aka propagate aka integrate) state estimate in-place.

Parameters

- **dt** – time to integrate over. The state time will be automatically incremented this amount unless you provide `destination_time`. Using `destination_time` may be preferable for prevention of roundoff error accumulation.
- **destination_time** – optional value to set continuous state time to after integration. If this is not provided, then *destination_frame_num* must be.
- **destination_frame_num** – optional value to set discrete state time to after integration. If this is not provided, then *destination_frame_num* must be.

innovation(*measurement*)
Compute and return the innovation that a measurement would induce if it were used for an update, but

don't actually perform the update. Assumes state and measurement are time-aligned. Useful for computing Chi^2 stats and likelihoods.

Parameters **measurement** – measurement

Returns Innovation mean and covariance of hypothetical update.

Return type tuple(torch.Tensor, torch.Tensor)

log_likelihood_of_update(*measurement*)
Compute and return the likelihood of a potential update, but don't actually perform the update. Assumes state and measurement are time- aligned. Useful for gating and calculating costs in assignment problems for data association.

Param measurement.

Returns Likelihood of hypothetical update.

update(*measurement*)
Use measurement to update state estimate in-place and return innovation. The innovation is useful, e.g., for evaluating filter consistency or updating model likelihoods when the EKFState is part of an IMMFState.

Param measurement.

Returns EKF State, Innovation mean and covariance.

23.5 Hashing

class LSH(*radius*)
Implements locality-sensitive hashing for low-dimensional euclidean space.

Allows to efficiently find neighbours of a point. Provides 2 guarantees:

- Difference between coordinates of points not returned by *nearby()* and input point is larger than radius.
- Difference between coordinates of points returned by *nearby()* and input point is smaller than 2 radius.

Example:

```
>>> radius = 1
>>> lsh = LSH(radius)
>>> a = torch.tensor([-0.51, -0.51]) # hash(a)=(-1,-1)
>>> b = torch.tensor([-0.49, -0.49]) # hash(a)=(0,0)
>>> c = torch.tensor([1.0, 1.0]) # hash(b)=(1,1)
>>> lsh.add('a', a)
>>> lsh.add('b', b)
>>> lsh.add('c', c)
>>> # even though c is within 2radius of a
>>> lsh.nearby('a') # doctest: +SKIP
{'b'}
>>> lsh.nearby('b') # doctest: +SKIP
{'a', 'c'}
>>> lsh.remove('b')
>>> lsh.nearby('a') # doctest: +SKIP
set()
```

Parameters **radius** (*float*) – Scaling parameter used in hash function. Determines the size of the neighbourhood.

add(*key*, *point*)
Adds (key, point) pair to the hash.

Parameters

- **key** – Key used identify point.
- **point** (*torch.Tensor*) – data, should be detached and on cpu.

remove(*key*)
Removes key and corresponding point from the hash.

Raises KeyError if key is not in hash.

Parameters **key** – key used to identify point.

nearby(*key*)
Returns a set of keys which are neighbours of the point identified by key.

Two points are nearby if difference of each element of their hashes is smaller than 2. In euclidean space, this corresponds to all points $\mathbf{p}$ where $|\mathbf{p}_k - (\mathbf{p_{key}})_k| < r$, and some points (all points not guaranteed) where $|\mathbf{p}_k - (\mathbf{p_{key}})_k| < 2r$.

Parameters **key** – key used to identify input point.

Returns a set of keys identifying neighbours of the input point.

Return type set

class ApproxSet(*radius*)
Queries low-dimensional euclidean space for approximate occupancy.

Parameters **radius** (*float*) – scaling parameter used in hash function. Determines the size of the bin. See *LSH* for details.

try_add(*point*)
Attempts to add point to set. Only adds there are no points in the point's bin.

Parameters **point** (*torch.Tensor*) – Point to be queried, should be detached and on cpu.

Returns True if point is successfully added, False if there is already a point in point's bin.

Return type bool

merge_points(*points*, *radius*)
Greedily merge points that are closer than given radius.

This uses *LSH* to achieve complexity that is linear in the number of merged clusters and quadratic in the size of the largest merged cluster.

Parameters

- **points** (*torch.Tensor*) – A tensor of shape (K,D) where K is the number of points and D is the number of dimensions.
- **radius** (*float*) – The minimum distance nearer than which points will be merged.

Returns A tuple (merged_points, groups) where merged_points is a tensor of shape (J,D) where J <= K, and groups is a list of tuples of indices mapping merged points to original points. Note that len(groups) == J and sum(len(group) for group in groups) == K.

Return type tuple

23.6 Measurements

class Measurement(*mean*, *cov*, *time=None*, *frame_num=None*)
Gaussian measurement interface.

Parameters

- **mean** – mean of measurement distribution.
- **cov** – covariance of measurement distribution.
- **time** – continuous time of measurement. If this is not provided, *frame_num* must be.
- **frame_num** – discrete time of measurement. If this is not provided, *time* must be.

dimension
Measurement space dimension access.

mean
Measurement mean (`z` in most Kalman Filtering literature).

cov
Noise covariance (`R` in most Kalman Filtering literature).

time
Continuous time of measurement.

frame_num
Discrete time of measurement.

geodesic_difference(*z1*, *z0*)
Compute and return the geodesic difference between 2 measurements. This is a generalization of the Euclidean operation `z1 - z0`.

Parameters

- **z1** – measurement.
- **z0** – measurement.

Returns Geodesic difference between `z1` and `z2`.

class DifferentiableMeasurement(*mean*, *cov*, *time=None*, *frame_num=None*)
Interface for Gaussian measurement for which Jacobians can be efficiently calculated, usu. analytically or by automatic differentiation.

jacobian(*x=None*)
Compute and return Jacobian (H) of measurement map (h) at target PV state `x` .

Parameters **x** – PV state. Use default argument `None` when the Jacobian is not state-dependent.

Returns Read-only Jacobian (H) of measurement map (h).

class PositionMeasurement(*mean*, *cov*, *time=None*, *frame_num=None*)
Full-rank Gaussian position measurement in Euclidean space.

Parameters

- **mean** – mean of measurement distribution.
- **cov** – covariance of measurement distribution.
- **time** – time of measurement.

jacobian(*x=None*)
Compute and return Jacobian (H) of measurement map (h) at target PV state `x` .

Parameters **x** – PV state. The default argument `None` may be used in this subclass since the Jacobian is not state-dependent.

Returns Read-only Jacobian (H) of measurement map (h).

CHAPTER 24

Indices and tables

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Python Module Index

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