General API quickstart

In [1]:

```
%matplotlib inline
import numpy as np
import theano.tensor as tt
import pymc3 as pm

import seaborn as sns
import matplotlib.pyplot as plt

sns.set_context('notebook')
plt.style.use('seaborn-darkgrid')
print('Running on PyMC3 v{}'.format(pm.__version__))
```

```
Running on PyMC3 v3.6
```

1. Model creation

Models in PyMC3 are centered around the `Model` class. It has references to all random variables (RVs) and computes the model logp and its gradients. Usually, you would instantiate it as part of a `with` context:

In [2]:

```
with pm.Model() as model:
    # Model definition
    pass
```

We discuss RVs further below but let's create a simple model to explore the `Model` class.

In [3]:

```
with pm.Model() as model:
    mu = pm.Normal('mu', mu=0, sigma=1)
    obs = pm.Normal('obs', mu=mu, sigma=1, observed=np.random.randn(100))
```

In [4]:

```
model.basic_RVs
```

Out[4]:

```
[mu, obs]
```

In [5]:

```
model.free_RVs
```

Out[5]:

```
[mu]
```

In [6]:

```
model.observed_RVs
```

Out[6]:

```
[obs]
```

In [7]:

```
model.logp({'mu': 0})
```

Out[7]:

```
array(-141.37324441)
```

Warning It's worth highlighting one of the counter-intuitive design choices with logp. The API makes the `logp` look like an attribute, when it actually puts together a function based on the current state of the model.

The current design is super maintainable, does terrible if the state stays constant, and great if the state keeps changing, for reasons of design we assume that `Model` isn't static, in fact it's best in our experience and avoids bad results.

If you need to use `logp` in an inner loop and it needs to be static, simply use something like `logp = model.logp` below. You can see the caching effect with the speed up below.

In [8]:

```
%timeit model.logp({mu: 0.1})
logp = model.logp
%timeit logp({mu: 0.1})
```

```
37.5 ms ± 356 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
12.3 µs ± 173 ns per loop (mean ± std. dev. of 7 runs, 100000 loops each)
```

2. Probability Distributions

Every probabilistic program consists of observed and unobserved Random Variables (RVs). Observed RVs are defined via likelihood distributions, while unobserved RVs are defined via prior distributions. In PyMC3, probability distributions are available from the main module space:

In [9]:

```
help(pm.Normal)
```

```
Help on class Normal in module pymc3.distributions.continuous:

class Normal(pymc3.distributions.distribution.Continuous)
 |  Normal(name, *args, **kwargs)
 |
 |  Univariate normal log-likelihood.
 |
 |  The pdf of this distribution is
 |
 |  .. math::
 |
 |     f(x \mid \mu, \tau) =
 |         \sqrt{\frac{\tau}{2\pi}}
 |         \exp\left\{ -\frac{\tau}{2} (x-\mu)^2 \right\}
 |
 |  Normal distribution can be parameterized either in terms of precision
 |  or standard deviation. The link between the two parametrizations is
 |  given by
 |
 |  .. math::
 |
 |     \tau = \dfrac{1}{\sigma^2}
 |
 |  .. plot::
 |
 |      import matplotlib.pyplot as plt
 |      import numpy as np
 |      import scipy.stats as st
 |      plt.style.use('seaborn-darkgrid')
 |      x = np.linspace(-5, 5, 1000)
 |      mus = [0., 0., 0., -2.]
 |      sigmas = [0.4, 1., 2., 0.4]
 |      for mu, sigma in zip(mus, sigmas):
 |          pdf = st.norm.pdf(x, mu, sigma)
 |          plt.plot(x, pdf, label=r'$\mu$ = {}, $\sigma$ = {}'.format(mu, sigma))
 |      plt.xlabel('x', fontsize=12)
```

```
 |      plt.xlabel('x', fontsize=12)
 |      plt.ylabel('f(x)', fontsize=12)
 |      plt.legend(loc=1)
 |      plt.show()
 |
 |  ========  ==========================================
 |  Support   :math:`x \in \mathbb{R}`
 |  Mean      :math:`\mu`
 |  Variance  :math:`\dfrac{1}{\tau}` or :math:`\sigma^2`
 |  ========  ==========================================
 |
 |  Parameters
 |  ----------
 |  mu : float
 |      Mean.
 |  sigma : float
 |      Standard deviation (sigma > 0) (only required if tau is not specified).
 |  tau : float
 |      Precision (tau > 0) (only required if sigma is not specified).
 |
 |  Examples
 |  --------
 |  .. code-block:: python
 |
 |      with pm.Model():
 |          x = pm.Normal('x', mu=0, sigma=10)
 |
 |      with pm.Model():
 |          x = pm.Normal('x', mu=0, tau=1/23)
 |
 |  Method resolution order:
 |      Normal
 |      pymc3.distributions.distribution.Continuous
 |      pymc3.distributions.distribution.Distribution
 |      builtins.object
 |
 |  Methods defined here:
 |
 |  __init__(self, mu=0, sigma=None, tau=None, sd=None, **kwargs)
 |      Initialize self.  See help(type(self)) for accurate signature.
 |
 |  logcdf(self, value)
 |
 |  logp(self, value)
 |      Calculate log-probability of Normal distribution at specified value.
 |
 |      Parameters
 |      ----------
 |      value : numeric
 |          Value(s) for which log-probability is calculated. If the log probabilities fo
r multiple
 |          values are desired the values must be provided in a numpy array or theano ten
sor
 |
 |      Returns
 |      -------
 |      TensorVariable
 |
 |  random(self, point=None, size=None)
 |      Draw random values from Normal distribution.
 |
 |      Parameters
 |      ----------
 |      point : dict, optional
 |          Dict of variable values on which random values are to be
 |          conditioned (uses default point if not specified).
 |      size : int, optional
 |          Desired size of random sample (returns one sample if not
 |          specified).
 |
 |      Returns
 |      -------
 |      array
```

```
 |      array
 |  
 |  ----------------------------------------------------------------------
 |  Methods inherited from pymc3.distributions.distribution.Distribution:
 |  
 |  __getnewargs__(self)
 |  
 |  __latex__ = _repr_latex_(self, name=None, dist=None)
 |      Magic method name for IPython to use for LaTeX formatting.
 |  
 |  default(self)
 |  
 |  get_test_val(self, val, defaults)
 |  
 |  getattr_value(self, val)
 |  
 |  logp_nojac(self, *args, **kwargs)
 |      Return the logp, but do not include a jacobian term for transforms.
 |      
 |      If we use different parametrizations for the same distribution, we
 |      need to add the determinant of the jacobian of the transformation
 |      to make sure the densities still describe the same distribution.
 |      However, MAP estimates are not invariant with respect to the
 |      parametrization, we need to exclude the jacobian terms in this case.
 |      
 |      This function should be overwritten in base classes for transformed
 |      distributions.
 |  
 |  logp_sum(self, *args, **kwargs)
 |      Return the sum of the logp values for the given observations.
 |      
 |      Subclasses can use this to improve the speed of logp evaluations
 |      if only the sum of the logp values is needed.
 |  
 |  ----------------------------------------------------------------------
 |  Class methods inherited from pymc3.distributions.distribution.Distribution:
 |  
 |  dist(*args, **kwargs) from builtins.type
 |  
 |  ----------------------------------------------------------------------
 |  Static methods inherited from pymc3.distributions.distribution.Distribution:
 |  
 |  __new__(cls, name, *args, **kwargs)
 |      Create and return a new object.  See help(type) for accurate signature.
 |  
 |  ----------------------------------------------------------------------
 |  Data descriptors inherited from pymc3.distributions.distribution.Distribution:
 |  
 |  __dict__
 |      dictionary for instance variables (if defined)
 |  
 |  __weakref__
 |      list of weak references to the object (if defined)
```

In the PyMC3 module, the structure for probability distributions looks like this:

pymc3.distributions

- continuous
- discrete
- timeseries
- mixture

In [10]:

```
dir(pm.distributions.mixture)
```

Out[10]:

```
['Discrete',
```

```
 'Distribution',
 'Iterable',
 'Mixture',
 'Normal',
 'NormalMixture',
 '_DrawValuesContext',
 '_DrawValuesContextBlocker',
 '__builtins__',
 '__cached__',
 '__doc__',
 '__file__',
 '__loader__',
 '__name__',
 '__package__',
 '__spec__',
 '_conversion_map',
 'all_discrete',
 'bound',
 'broadcast_distribution_samples',
 'draw_values',
 'generate_samples',
 'get_tau_sigma',
 'get_variable_name',
 'logsumexp',
 'np',
 'random_choice',
 'theano',
 'to_tuple',
 'tt']
```

Unobserved Random Variables

Every unobserved RV has the following calling signature: name (str), parameter keyword arguments. Thus, a normal prior can be defined in a model context like this:

In [11]:

```
with pm.Model():
    x = pm.Normal('x', mu=0, sigma=1)
```

As with the model, we can evaluate its logp:

In [12]:

```
x.logp({'x': 0})
```

Out[12]:

```
array(-0.91893853)
```

Observed Random Variables

Observed RVs are defined just like unobserved RVs but require data to be passed into the `observed` keyword argument:

In [13]:

```
with pm.Model():
    obs = pm.Normal('x', mu=0, sigma=1, observed=np.random.randn(100))
```

`observed` **supports lists,** `numpy.ndarray`**,** `theano` **and** `pandas` **data structures.**

Deterministic transforms

PyMC3 allows you to freely do algebra with RVs in all kinds of ways:

In [14]:

```
with pm.Model():
    x = pm.Normal('x', mu=0, sigma=1)
    y = pm.Gamma('y', alpha=1, beta=1)
    plus_2 = x + 2
    summed = x + y
    squared = x**2
    sined = pm.math.sin(x)
```

While these transformations work seamlessly, their results are not stored automatically. Thus, if you want to keep track of a transformed variable, you have to use `pm.Deterministic`:

In [15]:

```
with pm.Model():
    x = pm.Normal('x', mu=0, sigma=1)
    plus_2 = pm.Deterministic('x plus 2', x + 2)
```

Note that `plus_2` can be used in the identical way to above, we only tell PyMC3 to keep track of this RV for us.

Automatic transforms of bounded RVs

In order to sample models more efficiently, PyMC3 automatically transforms bounded RVs to be unbounded.

In [16]:

```
with pm.Model() as model:
    x = pm.Uniform('x', lower=0, upper=1)
```

When we look at the RVs of the model, we would expect to find `x` there, however:

In [17]:

```
model.free_RVs
```

Out[17]:

```
[x_interval__]
```

`x_interval__` represents `x` transformed to accept parameter values between -inf and +inf. In the case of an upper and a lower bound, a `LogOdd`s transform is applied. Sampling in this transformed space makes it easier for the sampler. PyMC3 also keeps track of the non-transformed, bounded parameters. These are common determinstics (see above):

In [18]:

```
model.deterministics
```

Out[18]:

```
[x]
```

When displaying results, PyMC3 will usually hide transformed parameters. You can pass the `include_transformed=True` parameter to many functions to see the transformed parameters that are used for sampling.

You can also turn transforms off:

In [19]:

```
with pm.Model() as model:
    x = pm.Uniform('x', lower=0, upper=1, transform=None)
```

```
print(model.free_RVs)
```

```
[x]
```

Or specify different transformation other than the default:

In [20]:

```
import pymc3.distributions.transforms as tr

with pm.Model() as model:
    # use the default log transformation
    x1 = pm.Gamma('x1', alpha=1, beta=1)
    # sepcified a different transformation
    x2 = pm.Gamma('x2', alpha=1, beta=1, transform=tr.log_exp_m1)

print('The default transformation of x1 is: ' + x1.transformation.name)
print('The user specified transformation of x2 is: ' + x2.transformation.name)
```

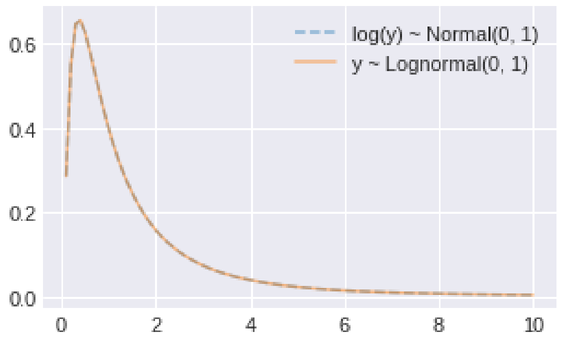
```
The default transformation of x1 is: log
The user specified transformation of x2 is: log_exp_m1
```

Transformed distributions and changes of variables

PyMC3 does not provide explicit functionality to transform one distribution to another. Instead, a dedicated distribution is usually created in consideration of optimising performance. However, users can still create transformed distribution by passing the inverse transformation to `transform` kwarg. Take the classical textbook example of LogNormal: $log(y) \sim \text{Normal}(\mu, \sigma)$

In [21]:

```
class Exp(tr.ElemwiseTransform):
    name = "exp"

    def backward(self, x):
        return tt.log(x)

    def forward(self, x):
        return tt.exp(x)

    def jacobian_det(self, x):
        return -tt.log(x)


with pm.Model() as model:
    x1 = pm.Normal('x1', 0., 1., transform=Exp())
    x2 = pm.Lognormal('x2', 0., 1.)

lognorm1 = model.named_vars['x1_exp__']
lognorm2 = model.named_vars['x2']

_, ax = plt.subplots(1, 1, figsize=(5, 3))
x = np.linspace(0., 10., 100)
ax.plot(
    x,
    np.exp(lognorm1.distribution.logp(x).eval()),
    '--',
    alpha=.5,
    label='log(y) ~ Normal(0, 1)')
ax.plot(
    x,
    np.exp(lognorm2.distribution.logp(x).eval()),
    alpha=.5,
    label='y ~ Lognormal(0, 1)')
plt.legend();
```

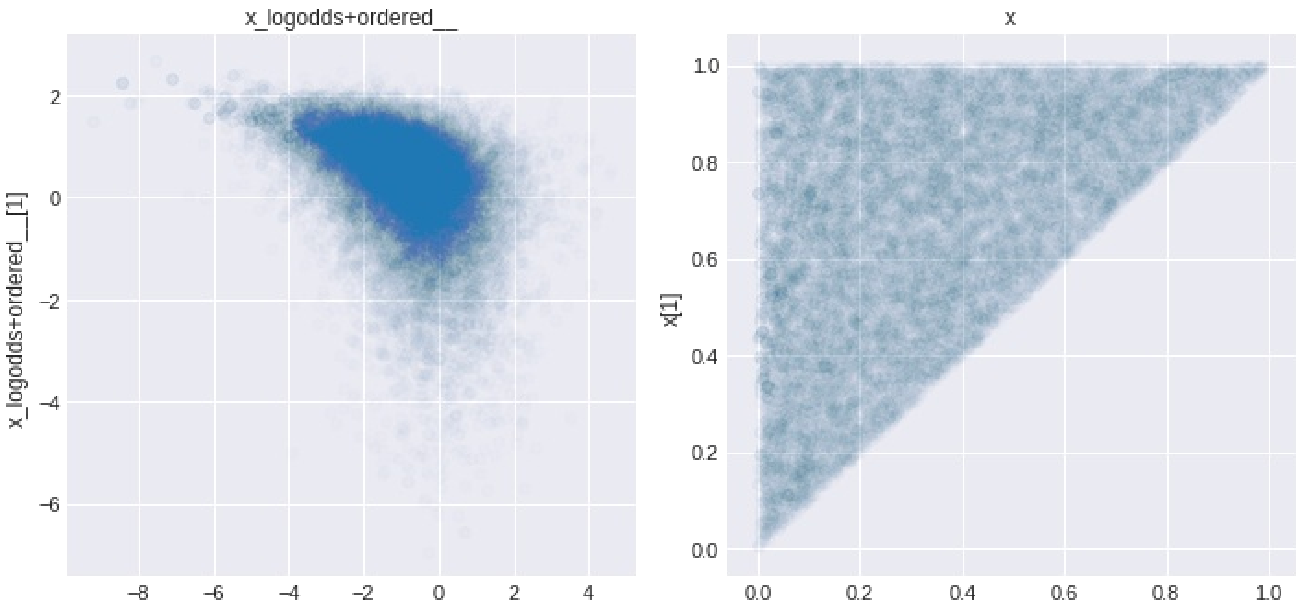


Notice from above that the named variable `x1_exp__` in the `model` is Lognormal distributed.
Using similar approach, we can create ordered RVs following some distribution. For example, we can combine the `ordered` transformation and `logodds` transformation using `Chain` to create a 2D RV that satisfy
x_1, x_2
$\sim \text{Uniform}$
$(0, 1)\ and\ x_1$
$< x_2$

In [22]:

```
Order = tr.Ordered()
Logodd = tr.LogOdds()
chain_tran = tr.Chain([Logodd, Order])

with pm.Model() as m0:
    x = pm.Uniform(
        'x', 0., 1., shape=2,
        transform=chain_tran,
        testval=[0.1, 0.9])
    trace = pm.sample(5000, tune=1000, progressbar=False)

_, ax = plt.subplots(1, 2, figsize=(10, 5))
for ivar, varname in enumerate(trace.varnames):
    ax[ivar].scatter(trace[varname][:, 0], trace[varname][:, 1], alpha=.01)
    ax[ivar].set_xlabel(varname + '[0]')
    ax[ivar].set_ylabel(varname + '[1]')
    ax[ivar].set_title(varname)
plt.tight_layout()
```

```
Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
Multiprocess sampling (4 chains in 4 jobs)
NUTS: [x]
The acceptance probability does not match the target. It is 0.8884785458718986, but shoul
d be close to 0.8. Try to increase the number of tuning steps.
There were 2 divergences after tuning. Increase `target_accept` or reparameterize.
```



x_logodds+ordered__[0] x[0]

Lists of RVs / higher-dimensional RVs

Above we have seen how to create scalar RVs. In many models, you want multiple RVs. There is a tendency (mainly inherited from PyMC 2.x) to create list of RVs, like this:

In [23]:

```
with pm.Model():
    x = [pm.Normal('x_{}'.format(i), mu=0, sigma=1) for i in range(10)] # bad
```

However, even though this works it is quite slow and not recommended. Instead, use the `shape` kwarg:

In [24]:

```
with pm.Model() as model:
    x = pm.Normal('x', mu=0, sigma=1, shape=10) # good
```

`x` is now a random vector of length 10. We can index into it or do linear algebra operations on it:

In [25]:

```
with model:
    y = x[0] * x[1] # full indexing is supported
    x.dot(x.T) # Linear algebra is supported
```

Initialization with test_values

While PyMC3 tries to automatically initialize models it is sometimes helpful to define initial values for RVs. This can be done via the `testval` kwarg:

In [26]:

```
with pm.Model():
    x = pm.Normal('x', mu=0, sigma=1, shape=5)

x.tag.test_value
```

Out[26]:

```
array([0., 0., 0., 0., 0.])
```

In [27]:

```
with pm.Model():
    x = pm.Normal('x', mu=0, sigma=1, shape=5, testval=np.random.randn(5))

x.tag.test_value
```

Out[27]:

```
array([-1.31813596, -0.44557099,  0.04482665, -1.8167009 ,  0.94796326])
```

This technique is quite useful to identify problems with model specification or initialization.

3. Inference

Once we have defined our model, we have to perform inference to approximate the posterior distribution. PyMC3 supports two broad classes of inference: sampling and variational inference.

3.1 Sampling

The main entry point to MCMC sampling algorithms is via the `pm.sample()` function. By default, this function

tries to auto-assign the right sampler(s) and auto-initialize if you don't pass anything.

In [28]:

```
with pm.Model() as model:
    mu = pm.Normal('mu', mu=0, sigma=1)
    obs = pm.Normal('obs', mu=mu, sigma=1, observed=np.random.randn(100))

    trace = pm.sample(1000, tune=500)
```

```
Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
Multiprocess sampling (4 chains in 4 jobs)
NUTS: [mu]
Sampling 4 chains: 100%|██████████| 6000/6000 [00:00<00:00, 7221.92draws/s]
```

As you can see, on a continuous model, PyMC3 assigns the NUTS sampler, which is very efficient even for complex models. PyMC3 also runs variational inference (i.e. ADVI) to find good starting parameters for the sampler. Here we draw 1000 samples from the posterior and allow the sampler to adjust its parameters in an additional 500 iterations. These 500 samples are discarded by default:

In [29]:

```
len(trace)
```

Out[29]:

```
1000
```

You can also run multiple chains in parallel using the `cores` kwarg:

In [30]:

```
with pm.Model() as model:
    mu = pm.Normal('mu', mu=0, sigma=1)
    obs = pm.Normal('obs', mu=mu, sigma=1, observed=np.random.randn(100))

    trace = pm.sample(cores=4)
```

```
Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
Multiprocess sampling (4 chains in 4 jobs)
NUTS: [mu]
Sampling 4 chains: 100%|██████████| 4000/4000 [00:00<00:00, 7935.96draws/s]
The acceptance probability does not match the target. It is 0.8978219346041421, but shoul
d be close to 0.8. Try to increase the number of tuning steps.
```

Note, that we are now drawing 2000 samples, 500 samples for 4 chains each. The 500 tuning samples are discarded by default.

In [31]:

```
trace['mu'].shape
```

Out[31]:

```
(2000,)
```

In [32]:

```
trace.nchains
```

Out[32]:

```
4
```

In [33]:

```
trace.get_values('mu', chains=1).shape # get values of a single chain
```

Out[33]:

```
(500,)
```

PyMC3, offers a variety of other samplers, found in `pm.step_methods`.

In [34]:

```python
list(filter(lambda x: x[0].isupper(), dir(pm.step_methods)))
```

Out[34]:

```
['BinaryGibbsMetropolis',
 'BinaryMetropolis',
 'CategoricalGibbsMetropolis',
 'CauchyProposal',
 'CompoundStep',
 'DEMetropolis',
 'ElemwiseCategorical',
 'EllipticalSlice',
 'HamiltonianMC',
 'LaplaceProposal',
 'Metropolis',
 'MultivariateNormalProposal',
 'NUTS',
 'NormalProposal',
 'PoissonProposal',
 'SMC',
 'Slice']
```

Commonly used step-methods besides NUTS are `Metropolis` and `Slice`. For almost all continuous models, `NUTS` should be preferred. There are hard-to-sample models for which `NUTS` will be very slow causing many users to use `Metropolis` instead. This practice, however, is rarely successful. NUTS is fast on simple models but can be slow if the model is very complex or it is badly initialized. In the case of a complex model that is hard for NUTS, Metropolis, while faster, will have a very low effective sample size or not converge properly at all. A better approach is to instead try to improve initialization of NUTS, or reparameterize the model.

For completeness, other sampling methods can be passed to sample:

In [35]:

```python
with pm.Model() as model:
    mu = pm.Normal('mu', mu=0, sigma=1)
    obs = pm.Normal('obs', mu=mu, sigma=1, observed=np.random.randn(100))

    step = pm.Metropolis()
    trace = pm.sample(1000, step=step)
```

```
Multiprocess sampling (4 chains in 4 jobs)
Metropolis: [mu]
Sampling 4 chains: 100%|██████████| 6000/6000 [00:00<00:00, 14925.91draws/s]
The number of effective samples is smaller than 25% for some parameters.
```

You can also assign variables to different step methods.

In [36]:

```python
with pm.Model() as model:
    mu = pm.Normal('mu', mu=0, sigma=1)
    sd = pm.HalfNormal('sd', sigma=1)
    obs = pm.Normal('obs', mu=mu, sigma=sd, observed=np.random.randn(100))

    step1 = pm.Metropolis(vars=[mu])
    step2 = pm.Slice(vars=[sd])
    trace = pm.sample(10000, step=[step1, step2], cores=4)
```

```
Multiprocess sampling (4 chains in 4 jobs)
CompoundStep
>Metropolis: [mu]
```

```
>Slice: [sd]
Sampling 4 chains: 100%|██████████| 42000/42000 [00:04<00:00, 8735.76draws/s]
The number of effective samples is smaller than 25% for some parameters.
```

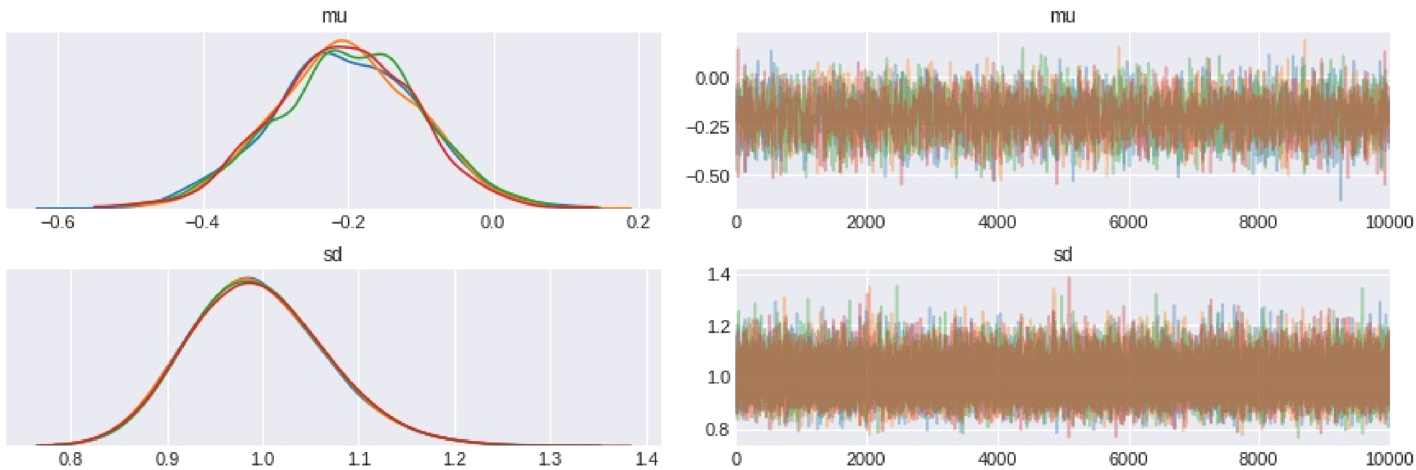
3.2 Analyze sampling results

The most common used plot to analyze sampling results is the so-called trace-plot:

In [37]:

```
pm.traceplot(trace);
```

```
/home/canyon/miniconda3/envs/pymc/lib/python3.7/site-packages/arviz/data/io_pymc3.py:56:
FutureWarning: arrays to stack must be passed as a "sequence" type such as list or tuple.
Support for non-sequence iterables such as generators is deprecated as of NumPy 1.16 and
will raise an error in the future.
  chain_likelihoods.append(np.stack(log_like))
```



Another common metric to look at is R-hat, also known as the Gelman-Rubin statistic:

In [38]:

```
pm.gelman_rubin(trace)
```

Out[38]:

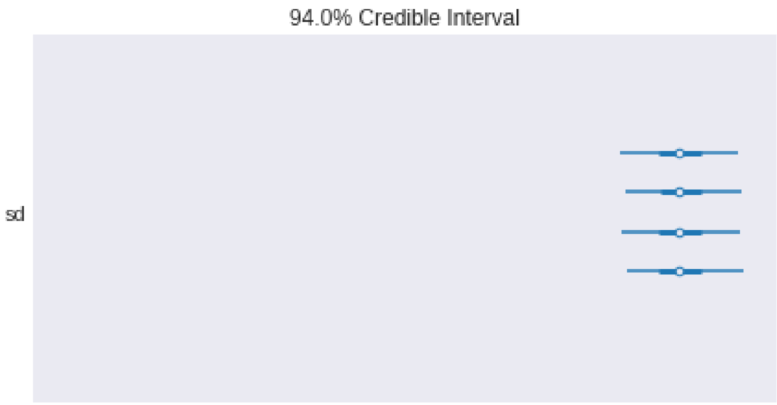
```
{'mu': 1.0006472993307545, 'sd': 0.9999963951762092}
```

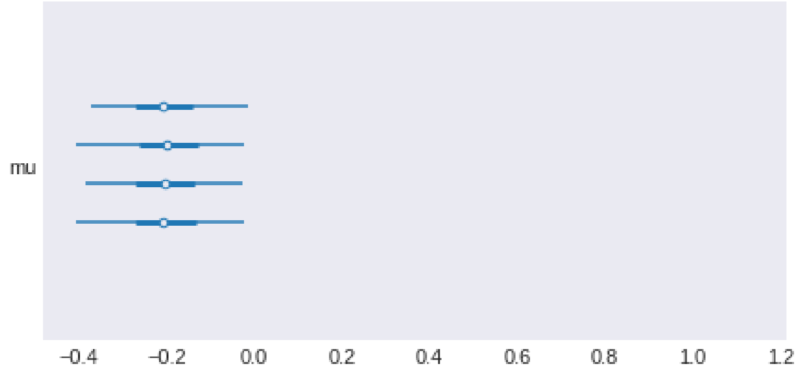
These are also part of the `forestplot`**:**

In [39]:

```
pm.forestplot(trace);
```

```
/home/canyon/miniconda3/envs/pymc/lib/python3.7/site-packages/arviz/data/io_pymc3.py:56:
FutureWarning: arrays to stack must be passed as a "sequence" type such as list or tuple.
Support for non-sequence iterables such as generators is deprecated as of NumPy 1.16 and
will raise an error in the future.
  chain_likelihoods.append(np.stack(log_like))
```

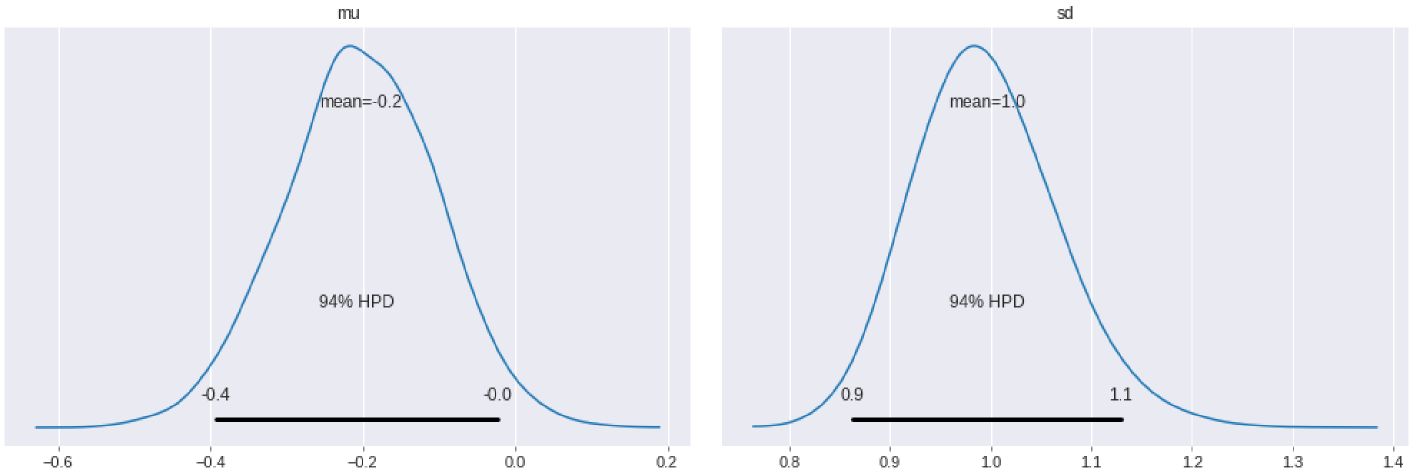




Finally, for a plot of the posterior that is inspired by the book [Doing Bayesian Data Analysis](), you can use the:

In [40]:

```
pm.plot_posterior(trace);
```

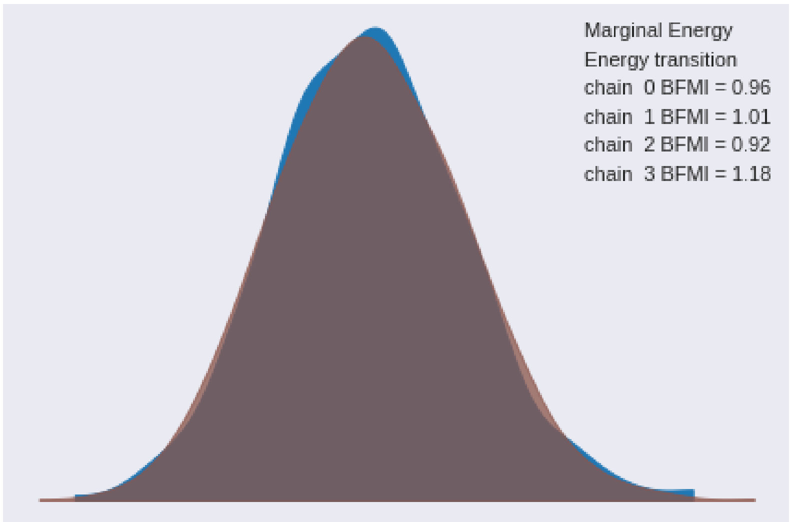


For high-dimensional models it becomes cumbersome to look at all parameter's traces. When using `NUTS` we can look at the energy plot to assess problems of convergence:

In [41]:

```
with pm.Model() as model:
    x = pm.Normal('x', mu=0, sigma=1, shape=100)
    trace = pm.sample(cores=4)

pm.energyplot(trace);
```

```
Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
Multiprocess sampling (4 chains in 4 jobs)
NUTS: [x]
Sampling 4 chains: 100%|██████████| 4000/4000 [00:01<00:00, 2280.44draws/s]
```



For more information on sampler stats and the energy plot, see here. For more information on identifying sampling problems and what to do about them, see here.

3.3 Variational inference

PyMC3 supports various Variational Inference techniques. While these methods are much faster, they are often also less accurate and can lead to biased inference. The main entry point is `pymc3.fit()`.

In [42]:

```
with pm.Model() as model:
    mu = pm.Normal('mu', mu=0, sigma=1)
    sd = pm.HalfNormal('sd', sigma=1)
    obs = pm.Normal('obs', mu=mu, sigma=sd, observed=np.random.randn(100))

    approx = pm.fit()
```

```
Average Loss = 138.84: 100%|██████████| 10000/10000 [00:01<00:00, 6462.56it/s]
Finished [100%]: Average Loss = 138.83
```

The returned `Approximation` object has various capabilities, like drawing samples from the approximated posterior, which we can analyse like a regular sampling run:

In [43]:

```
approx.sample(500)
```

Out[43]:

```
<MultiTrace: 1 chains, 500 iterations, 3 variables>
```

The `variational` submodule offers a lot of flexibility in which VI to use and follows an object oriented design. For example, full-rank ADVI estimates a full covariance matrix:

In [44]:

```
mu = pm.floatX([0., 0.])
cov = pm.floatX([[1, .5], [.5, 1.]])
with pm.Model() as model:
    pm.MvNormal('x', mu=mu, cov=cov, shape=2)
    approx = pm.fit(method='fullrank_advi')
```

```
  0%|          | 0/10000 [00:00<?, ?it/s]/home/canyon/miniconda3/envs/pymc/lib/python3.7/
site-packages/theano/tensor/subtensor.py:2339: FutureWarning: Using a non-tuple sequence
for multidimensional indexing is deprecated; use `arr[tuple(seq)]` instead of `arr[seq]`.
In the future this will be interpreted as an array index, `arr[np.array(seq)]`, which wil
l result either in an error or a different result.
  out[0][inputs[2:]] = inputs[1]
/home/canyon/miniconda3/envs/pymc/lib/python3.7/site-packages/theano/tensor/basic.py:6611
: FutureWarning: Using a non-tuple sequence for multidimensional indexing is deprecated;
use `arr[tuple(seq)]` instead of `arr[seq]`. In the future this will be interpreted as an
array index, `arr[np.array(seq)]`, which will result either in an error or a different re
sult.
  result[diagonal_slice] = x
/home/canyon/miniconda3/envs/pymc/lib/python3.7/site-packages/theano/tensor/subtensor.py:
2197: FutureWarning: Using a non-tuple sequence for multidimensional indexing is deprecat
ed; use `arr[tuple(seq)]` instead of `arr[seq]`. In the future this will be interpreted a
s an array index, `arr[np.array(seq)]`, which will result either in an error or a differe
nt result.
  rval = inputs[0].__getitem__(inputs[1:])
Average Loss = 0.0068883: 100%|██████████| 10000/10000 [00:03<00:00, 2795.26it/s]
Finished [100%]: Average Loss = 0.0065707
```

An equivalent expression using the object-oriented interface is:

In [45]:

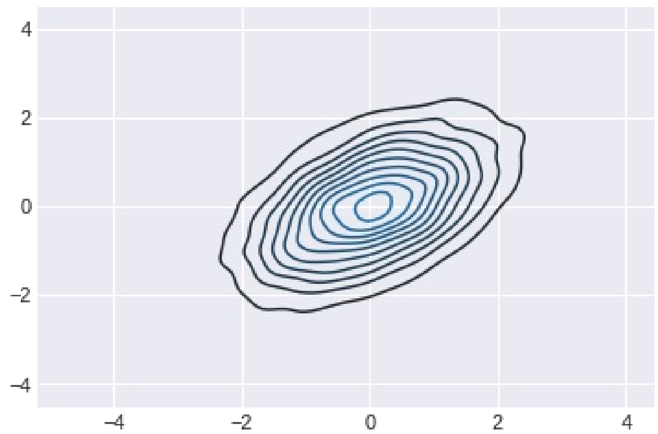
```
with pm.Model() as model:
    pm.MvNormal('x', mu=mu, cov=cov, shape=2)
    approx = pm.FullRankADVI().fit()
```

```
Average Loss = 0.01127: 100%|██████████| 10000/10000 [00:03<00:00, 2541.45it/s]
Finished [100%]: Average Loss = 0.011343
```

In [46]:

```
plt.figure()
trace = approx.sample(10000)
sns.kdeplot(trace['x'][:, 0], trace['x'][:, 1]);
```

```
/home/canyon/miniconda3/envs/pymc/lib/python3.7/site-packages/theano/tensor/subtensor.py:
2339: FutureWarning: Using a non-tuple sequence for multidimensional indexing is deprecat
ed; use `arr[tuple(seq)]` instead of `arr[seq]`. In the future this will be interpreted a
s an array index, `arr[np.array(seq)]`, which will result either in an error or a differe
nt result.
  out[0][inputs[2:]] = inputs[1]
```



Stein Variational Gradient Descent (SVGD) uses particles to estimate the posterior:

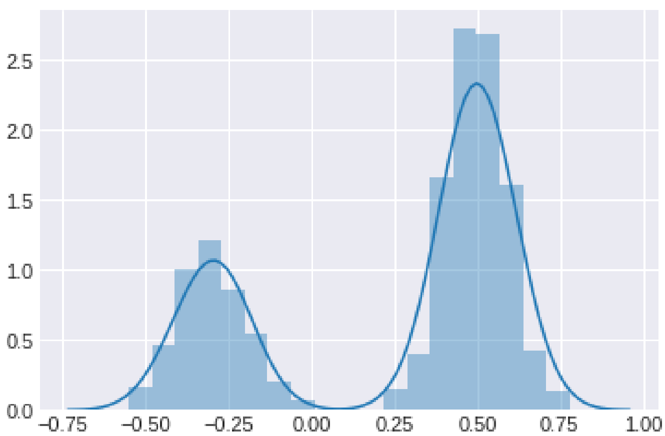
In [47]:

```
w = pm.floatX([.2, .8])
mu = pm.floatX([-.3, .5])
sd = pm.floatX([.1, .1])
with pm.Model() as model:
    pm.NormalMixture('x', w=w, mu=mu, sigma=sd)
    approx = pm.fit(method=pm.SVGD(n_particles=200, jitter=1.))
```

```
100%|██████████| 10000/10000 [00:41<00:00, 242.58it/s]
```

In [48]:

```
plt.figure()
trace = approx.sample(10000)
sns.distplot(trace['x']);
```



For more information on variational inference, see [these examples](#).

4. Posterior Predictive Sampling

The `sample_posterior_predictive()` function performs prediction on hold-out data and posterior predictive checks.

In [49]:

```
data = np.random.randn(100)
with pm.Model() as model:
    mu = pm.Normal('mu', mu=0, sigma=1)
    sd = pm.HalfNormal('sd', sigma=1)
    obs = pm.Normal('obs', mu=mu, sigma=sd, observed=data)

    trace = pm.sample()
```

```
Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
Multiprocess sampling (4 chains in 4 jobs)
NUTS: [sd, mu]
Sampling 4 chains: 100%|██████████| 4000/4000 [00:00<00:00, 6391.82draws/s]
```

In [66]:

```
with model:
    post_pred = pm.sample_posterior_predictive(trace, samples=500)
```

```
100%|██████████| 500/500 [00:00<00:00, 4278.10it/s]
```

`sample_posterior_predictive()` returns a dict with a key for every observed node:

In [67]:

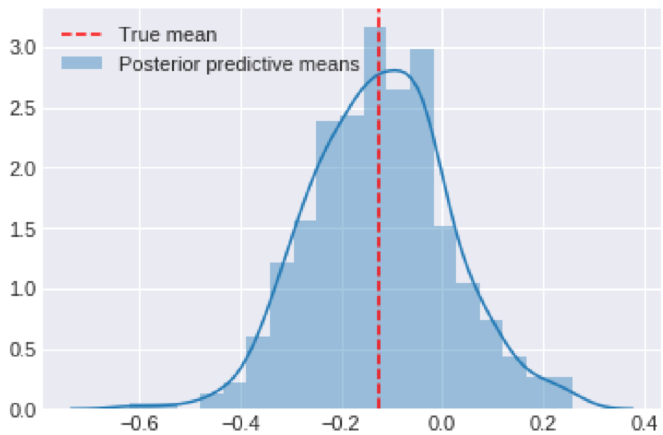
```
post_pred['obs'].shape
```

Out[67]:

```
(500, 100)
```

In [69]:

```
fig, ax = plt.subplots()
sns.distplot(post_pred['obs'].mean(axis=1), label='Posterior predictive means', ax=ax)
ax.axvline(data.mean(), ls='--', color='r', label='True mean')
ax.legend();
```



4.1 Predicting on hold-out data

In many cases you want to predict on unseen / hold-out data. This is especially relevant in Probabilistic Machine Learning and Bayesian Deep Learning. While we plan to improve the API in this regard, this can currently be achieved with a `theano.shared` variable. These are theano tensors whose values can be changed later.

Otherwise they can be passed into PyMC3 just like any other numpy array or tensor.

This distinction is significant since internally all models in PyMC3 are giant symbolic expressions. When you pass data directly into a model, you are giving Theano permission to treat this data as a constant and optimize it away as it sees fit. If you need to change this data later you might not have a way to point at it in the symbolic expression. Using `theano.shared` offers a way to point to a place in that symbolic expression, and change what is there.

In [70]:

```
import theano

x = np.random.randn(100)
y = x > 0

x_shared = theano.shared(x)
y_shared = theano.shared(y)

with pm.Model() as model:
    coeff = pm.Normal('x', mu=0, sigma=1)
    logistic = pm.math.sigmoid(coeff * x_shared)
    pm.Bernoulli('obs', p=logistic, observed=y_shared)
    trace = pm.sample()
```

```
Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
Multiprocess sampling (4 chains in 4 jobs)
NUTS: [x]
Sampling 4 chains: 100%|██████████| 4000/4000 [00:00<00:00, 6878.69draws/s]
The acceptance probability does not match the target. It is 0.8860942205889539, but shoul
d be close to 0.8. Try to increase the number of tuning steps.
```

Now assume we want to predict on unseen data. For this we have to change the values of `x_shared` and `y_shared`. Theoretically we don't need to set `y_shared` as we want to predict it but it has to match the shape of `x_shared`.

In [71]:

```
x_shared.set_value([-1, 0, 1.])
y_shared.set_value([0, 0, 0]) # dummy values

with model:
    post_pred = pm.sample_posterior_predictive(trace, samples=500)
```

```
100%|██████████| 500/500 [00:03<00:00, 157.63it/s]
```

In [72]:

```
post_pred['obs'].mean(axis=0)
```

Out[72]:

```
array([0.014, 0.514, 0.988])
```