Probabilistic Programming with Pyro

UBER AI Labs

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Why Pyro?

Why probabilistic modeling? To correctly capture uncertainty in models and predictions, for unsupervised and semi-supervised learning, and to provide AI systems with declarative prior knowledge.

Why (universal) probabilistic programs? To provide a clear and high-level, but complete, language for specifying complex models.

Why deep probabilistic models? To learn generative knowledge from data and reify knowledge of how to do inference.

Why inference by optimization? To enable scaling to large data and leverage advances in modern optimization and variational inference.

What is Pyro?

Pyro models are functions with:

- Arbitrary Python and PyTorch code
- Pyro primitives for: sampling, observation, and learnable parameters

Pyro automates inference:

- Variational method takes a model and an inference model (or guide) and optimizes Evidence Lower Bound.
- Tools to reduce the variance of gradient estimates, handle mini-batching, etc.
- Can also do exact inference, importance sampling, and coming soon: MCMC, SMC.

Design Principles

Universal: Pyro can represent any computable probability distribution.

Scalable: Pyro scales to large data sets with little overhead.

Minimal: Pyro is implemented with a small core of powerful, composable abstractions.

Flexible: Pyro aims for automation when you want it, control when you need it.

Pyro primitives

```
pyro.sample("my_sample", dist.normal, mu, sigma)
```

```
Variable containing:
-0.3098
[torch.FloatTensor of size 1]
```

```
pyro.sample("my_observed_sample", dist.normal, mu, sigma,
            obs=Variable(torch.ones(1)))
```

Makes sense only in the context of an inference algorithm!

```
pyro.param("mu", Variable(torch.ones(1), requires_grad=True))
```

```
Variable containing:
 1
[torch.FloatTensor of size 1]
```

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Variational autoencoder (VAE): model

register parameters in decoder with Pyro

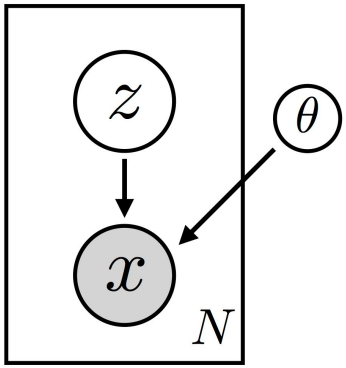
sample latent code

decode latent code

return sampled image

```
def model():
    pyro.module("decoder", nn_decoder)
    z = pyro.sample("z", dist.normal, ng_zeros(20), ng_ones(20))
    bern_prob = nn_decoder(z)
    return pyro.sample("x", dist.bernoulli, bern_prob)


nn_decoder = nn.Sequential(
    nn.Linear(20, 100),
    nn.Softplus(),
    nn.Linear(100, 784),
    nn.Sigmoid()
)
```



Auto-Encoding Variational Bayes,
Diederik P Kingma, Max Welling

Stochastic Backpropagation and Approximate Inference in Deep Generative Models,
Danilo Jimenez Rezende, Shakir Mohamed, Daan Wierstra

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Variational autoencoder (VAE): model

register parameters in decoder with Pyro

sample latent code

decode latent code

***observe* image**

```
def model(x):
    pyro.module("decoder", nn_decoder)
    z = pyro.sample("z", dist.normal, ng_zeros(20), ng_ones(20))
    bern_prob = nn_decoder(z)
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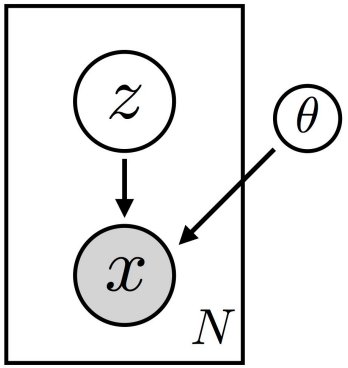

Auto-Encoding Variational Bayes,
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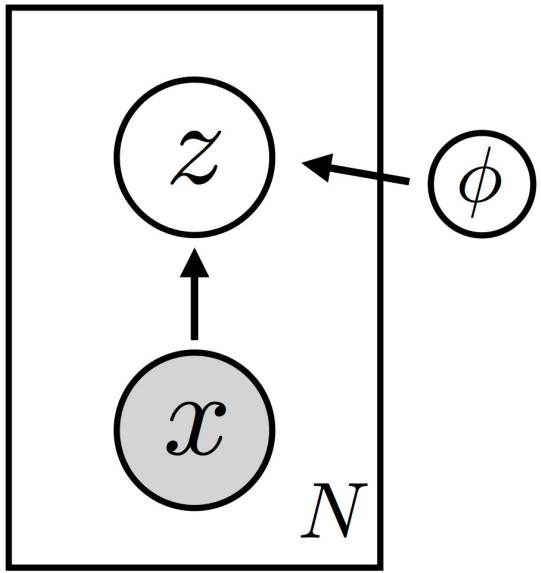
VAE: inference

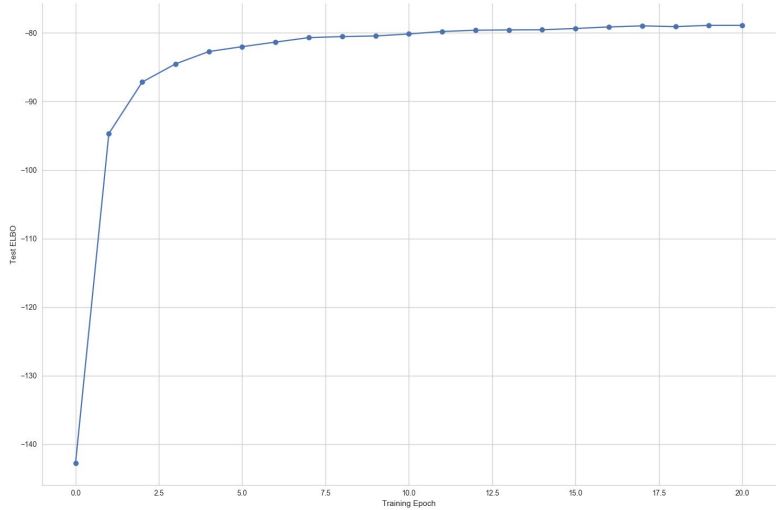
```
def guide(x):
    # nn_encoder is another neural network,
    # that takes in an image x and outputs the parameters
    # of a distribution over a latent code z given x
    pyro.module("encoder", nn_encoder)
    mu_z, sig_z = nn_encoder(x)
    return pyro.sample("z", dist.normal, mu_z, sig_z)
```



VAE: inference

```
svi = pyro.infer.SVI(model=model,
                     guide=guide,
                     optim=pyro.optim.Adam({"lr": 0.001}),
                     loss="ELBO")
```

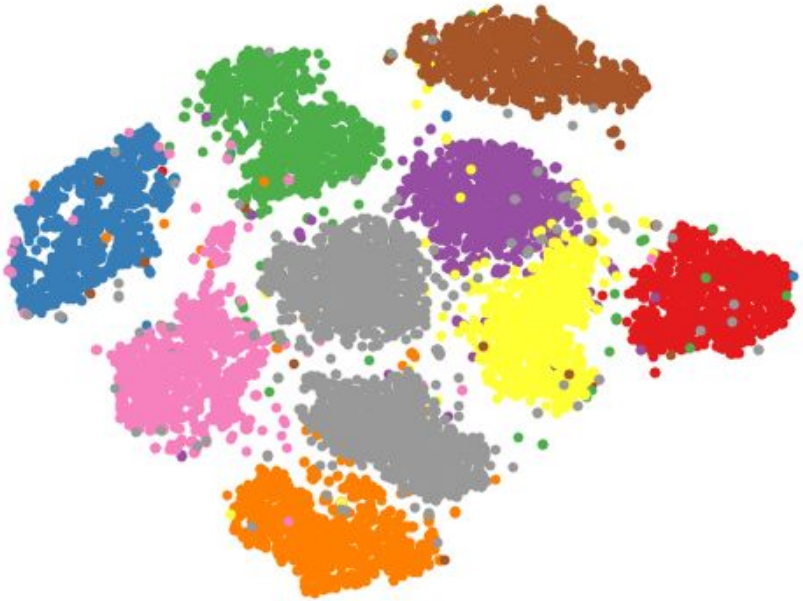
```
losses = []
for batch in batches:
    losses.append(svi.step(batch))
```



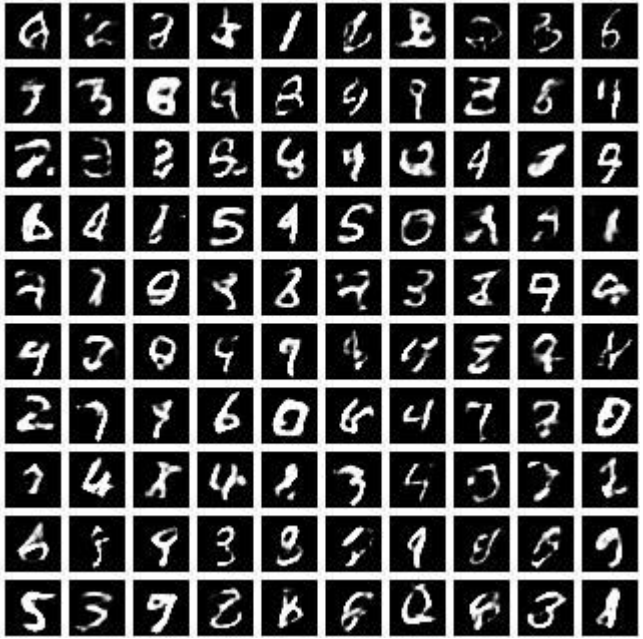
progress on elbo during training

VAE: results

latent embedding



samples from the generative model



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VAE: all together

```
def model(x):
    pyro.module("decoder", nn_decoder)
    z = pyro.sample("z", dist.normal, ng_zeros(20), ng_ones(20))
    bern_prob = nn_decoder(z)
    return pyro.sample("x", dist.bernoulli, bern_prob, obs=x)
```

```
def guide(x):
    pyro.module("encoder", nn_encoder)
    mu_z, sig_z = nn_encoder(x)
    return pyro.sample("z", dist.normal, mu_z, sig_z)
```

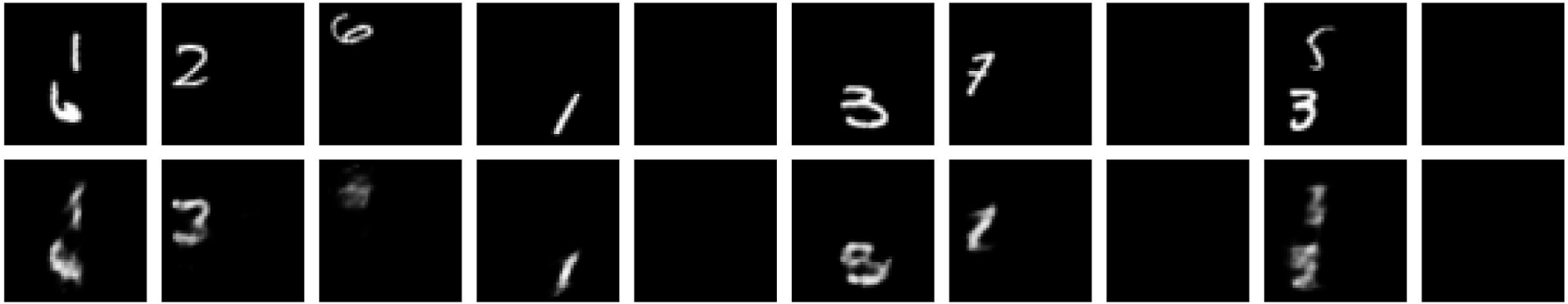
```
svi = pyro.infer.SVI(model=model,
                     guide=guide,
                     optim=pyro.optim.Adam({"lr": 0.001}),
                     loss="ELBO")
```

Cool.

With the VAE in hand we can now tackle all unsupervised learning problems, right?

VAE: Multi-MNIST

test set reconstructions (0/1/2 digits)

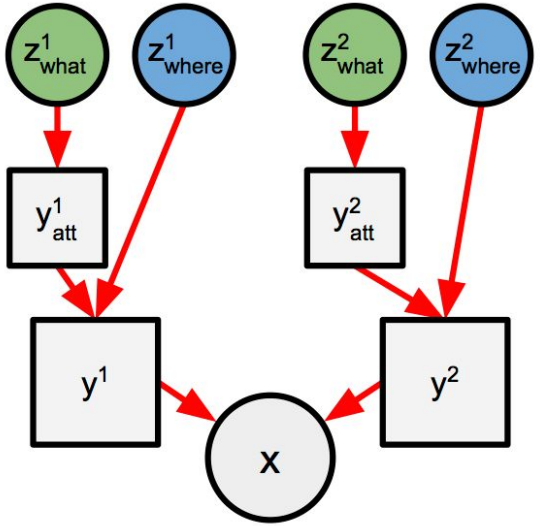


not so great... maybe we need a more sophisticated model?

Attend-Infer-Repeat in Pyro

Let's build in an abstract **object concept**:

- scenes are made of **some number** of things
- each thing has a **what**
- and a **where**



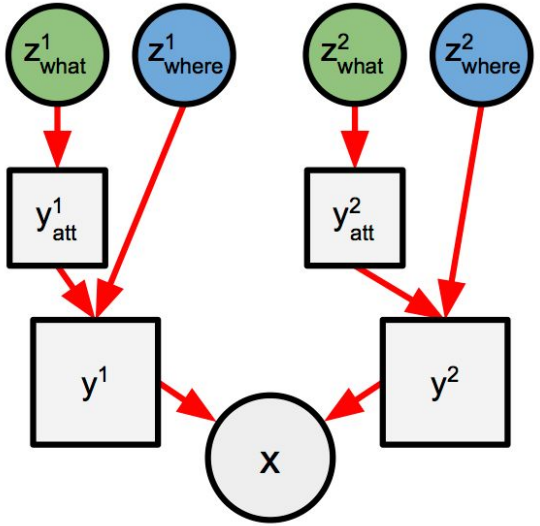
reproduced from reference

Attend, Infer, Repeat: Fast Scene Understanding with Generative Models (arXiv:1603.08575),
S.M. Ali Eslami, Nicolas Heess, Theophane Weber, Yuval Tassa, David Szepesvari, Koray Kavukcuoglu, Geoffrey E. Hinton

Attend-Infer-Repeat in Pyro

Let's build in an abstract **object concept**:

- scenes are made of **some number** of things
- each thing has a **what** (VAE-style appearance model)
- and a **where** (location and size to place into image)



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Interlude: recursion, random control flow, and other awesomeness

the geometric distribution defined recursively with bernoulli random trials

```
def geom(num_trials=0):
    p = Variable(torch.Tensor([0.5]))
    x = pyro.sample('x{}'.format(num_trials), dist.bernoulli, p)
    if x.data[0] == 1:
        return num_trials
    else:
        return geom(num_trials + 1)
```

dynamically named random variable

different executions of geom() can have different numbers of random variables

Back to AIR: A recursive prior for images

first we need to define a prior over a single object in the image

```
def prior_step(t):
    # Sample object pose. This is a 3-dimensional vector representing x,y position and size.
    z_where = pyro.sample('z_where_{}'.format(t),
                          dist.normal,
                          z_where_prior_mu, z_where_prior_sigma)

    # Sample object code. This is a 50-dimensional vector.
    z_what = pyro.sample('z_what_{}'.format(t),
                         dist.normal,
                         z_what_prior_mu, z_what_prior_sigma)

    y_att = decode(z_what)                  # Map latent code to pixel space using the neural network.

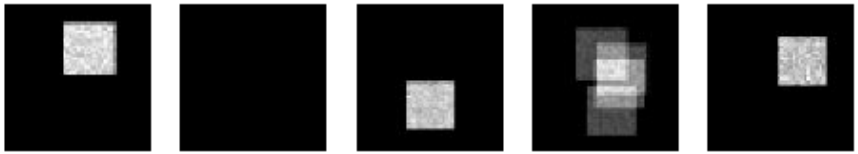
    y = object_to_image(z_where, y_att)     # Position/scale object within larger image
                                            # using (differentiable) spatial transformations
    return y
```

Back to AIR: A recursive prior for images

canvas (initially empty)

```
def geom_image_prior(x, step=0):
    p = Variable(torch.Tensor([0.5]))
    i = pyro.sample('i{}'.format(step), dist.bernoulli, p)
    if i.data[0] == 1:
        return x
    else:
        x = x + prior_step(step)
        return geom_image_prior(x, step + 1)
```

add sampled object to canvas



samples from prior

AIR: Inference

consume hidden state from previous step to inform sampling in this step

controls when to stop recursion

sample latent code for image patch

```
def guide_step(t, data, prev):

    rnn_input = torch.cat((data, prev.z_where, prev.z_what, prev.z_pres), 1)
    h, c = rnn(rnn_input, (prev.h, prev.c))
    z_pres_p, z_where_mu, z_where_sigma = predict(h)

    z_pres = pyro.sample('z_pres_{}'.format(t),
                         dist.bernoulli, z_pres_p * prev.z_pres)

    z_where = pyro.sample('z_where_{}'.format(t),
                          dist.normal, z_where_mu, z_where_sigma)

    x_att = image_to_object(z_where, data)  # Crop a small window from the input.

    # Compute the parameter of the distribution over z_what
    # by passing the window through the encoder network.
    z_what_mu, z_what_sigma = encode(x_att)

    z_what = pyro.sample('z_what_{}'.format(t),
                                 dist.normal, z_what_mu, z_what_sigma)

    return # values for next step
```

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Variance Reduction

because we have discrete random variables a naive ELBO gradient estimator will contain terms of the form

$$\nabla_\phi \log q(z_{\text{bern}}) \times \text{ELBO}$$

to reduce variance we instead use a gradient estimator with terms of the form

$$\nabla_\phi \log q(z_{\text{bern}}) \times (D_{z_{\text{bern}}} - b)$$

neural baseline

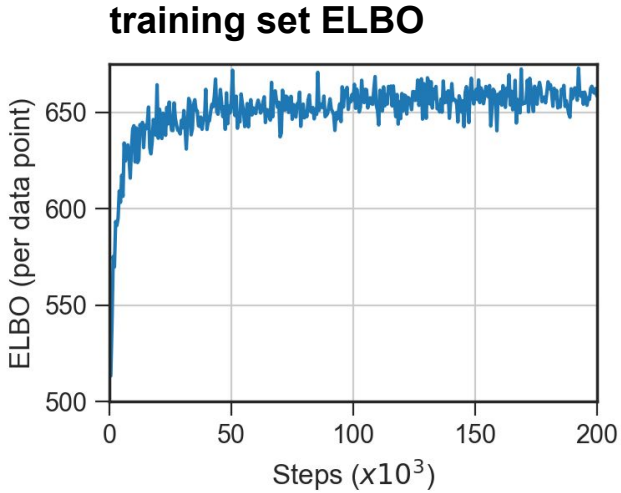
downstream cost

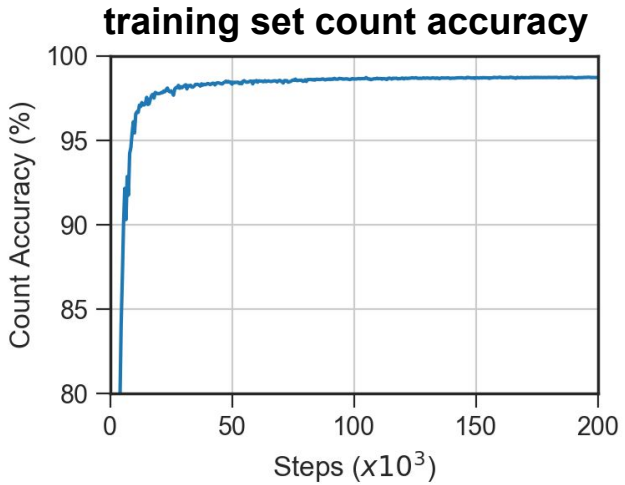
in Pyro invoking the improved estimator is simple:

```
pyro.sample('z_bern', dist.bernoulli, ..., baseline=dict(baseline_value=b))
svi = SVI(air.model, air.guide, ..., loss='ELBO', trace_graph=True)
```

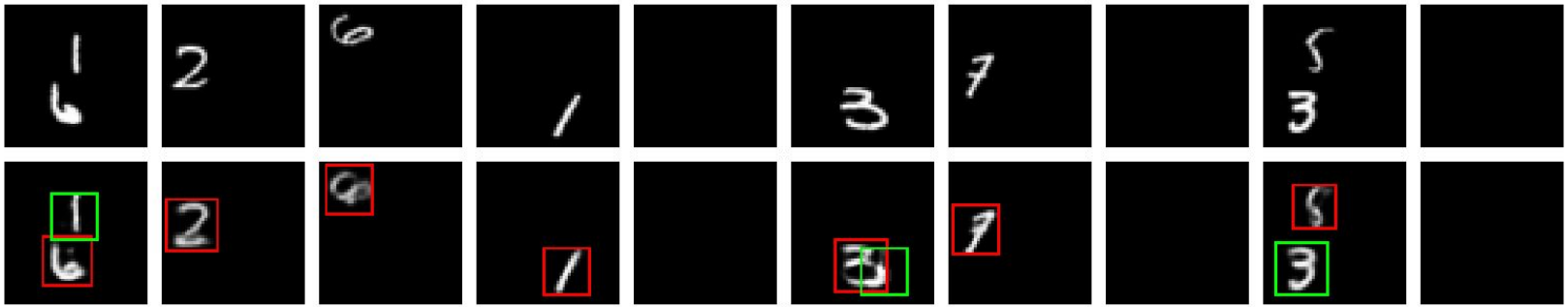

Neural Variational Inference and Learning in Belief Networks,
Andriy Mnih, Karol Gregor

AIR: Results





test set reconstructions



Reusing components for image reconstruction

arguments to guide

```
import pyro.poutine as poutine
```

the trace contains all the random variables sampled by the guide

```
trace = poutine.trace(air.guide).get_trace(examples_to_viz, None)
```

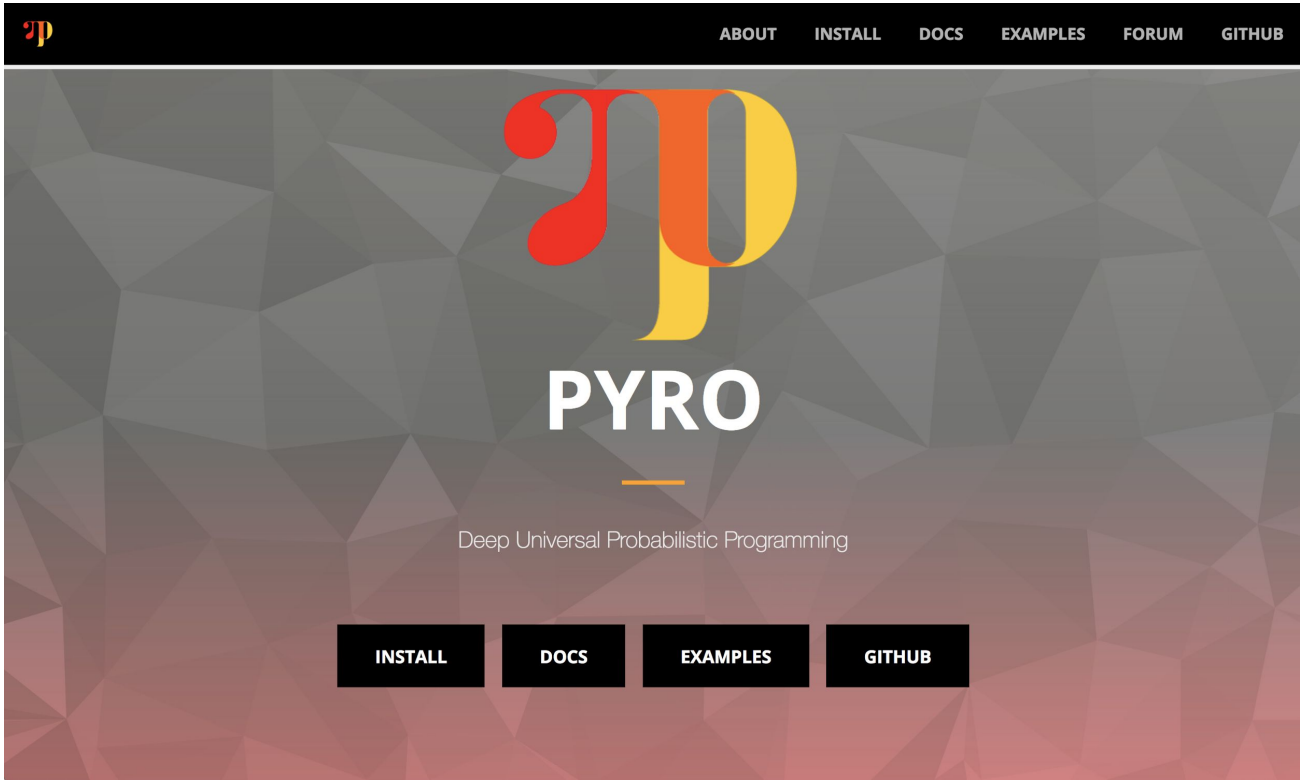
replay the prior against the trace to get the return values of air.prior

```
z, recons = poutine.replay(air.prior, trace)(examples_to_viz.size(0))
```

argument to prior

- note that air.prior is the entire model except for the observation noise
- this trace + replay paradigm is also how the backend constructs the ELBO

pyro.ai



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