Pyro

Deep Probabilistic Programming 101: The Variational Autoencoder

UBER AI Labs

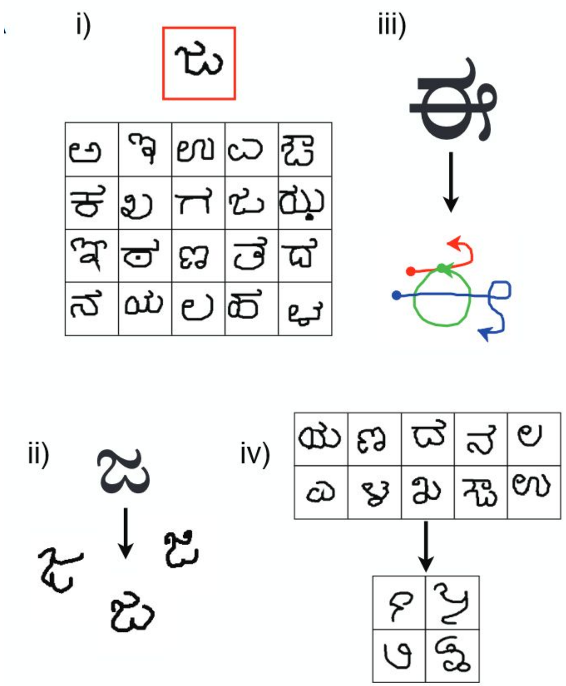
In this tutorial:

1. Introduction to deep generative models and model learning
2. Implementing a simple deep generative model with Pyro
3. Performing variational inference with model learning in the VAE
4. A brief look at how inference algorithms are implemented in Pyro

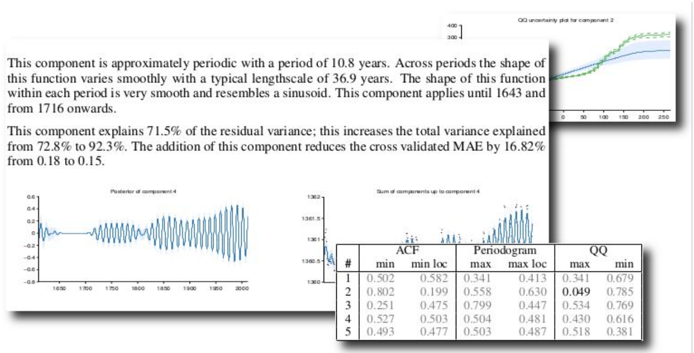
Based on the following Pyro tutorials:

- Variational Autoencoders: http://pyro.ai/examples/vae.html
- Intro to SVI: http://pyro.ai/examples/svi_part_i.html

Probabilistic Modelling in AI: Frontiers

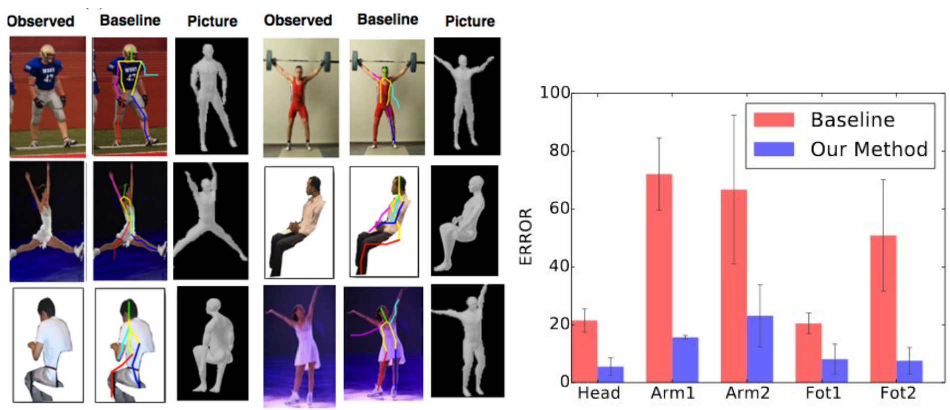


Human-level concept learning through probabilistic program induction, Lake et al.



#	ACF min	ACF min loc	Periodogram max	Periodogram max loc	QQ max	QQ min
1	0.502	0.582	0.341	0.413	0.341	0.679
2	0.802	0.199	0.558	0.630	0.049	0.785
3	0.251	0.475	0.799	0.447	0.534	0.769
4	0.527	0.503	0.504	0.481	0.430	0.616
5	0.493	0.477	0.503	0.487	0.518	0.381

Automatic Construction and Natural-Language Description of Nonparametric Regression Models, Lloyd et al.



Picture: A Probabilistic Programming Language for Scene Perception, Kulkarni et al.

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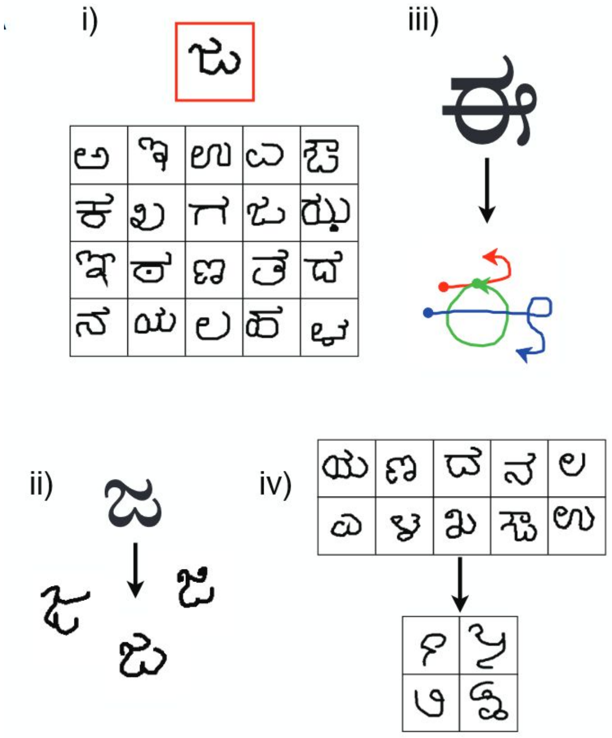
Probabilistic Modelling in AI: Frontiers



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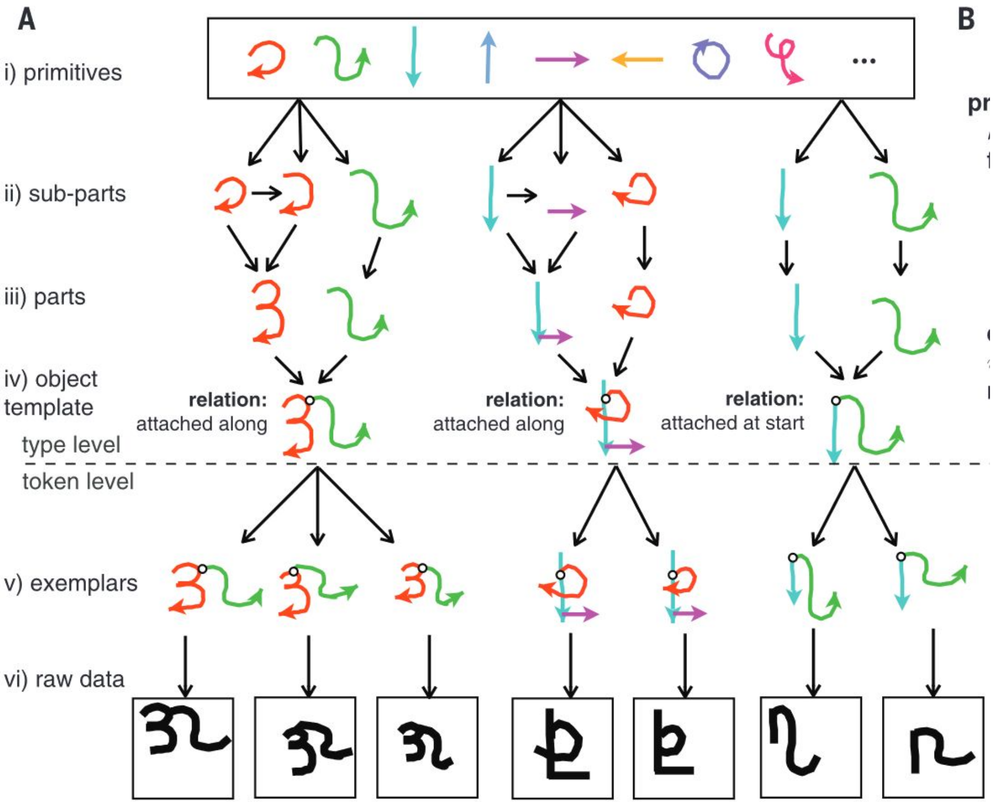
Probabilistic Modelling in AI: Frontiers



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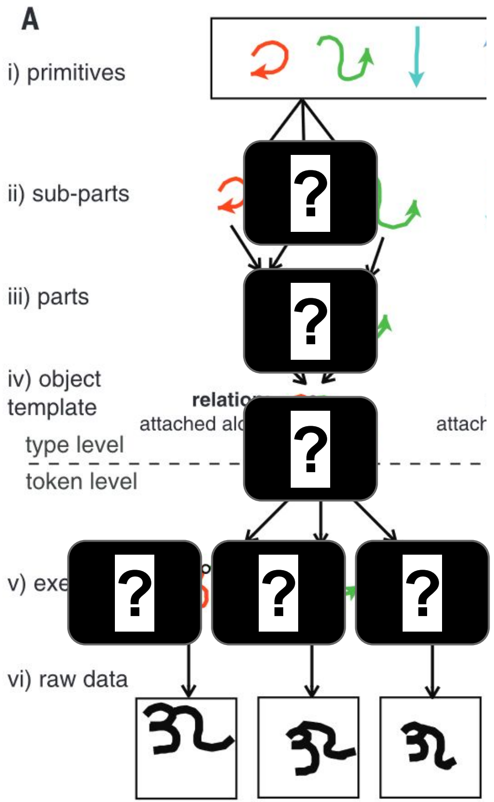
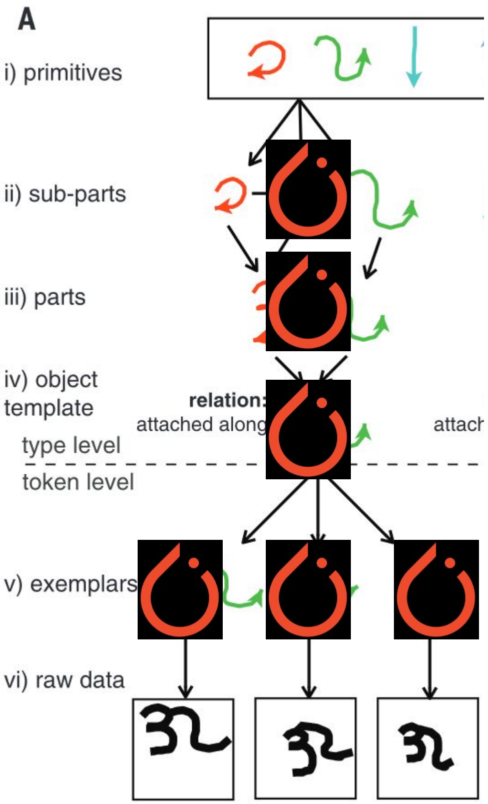
Human-level concept learning through probabilistic program induction, Lake et al.

What if we can't write down a good model?



Deep generative models



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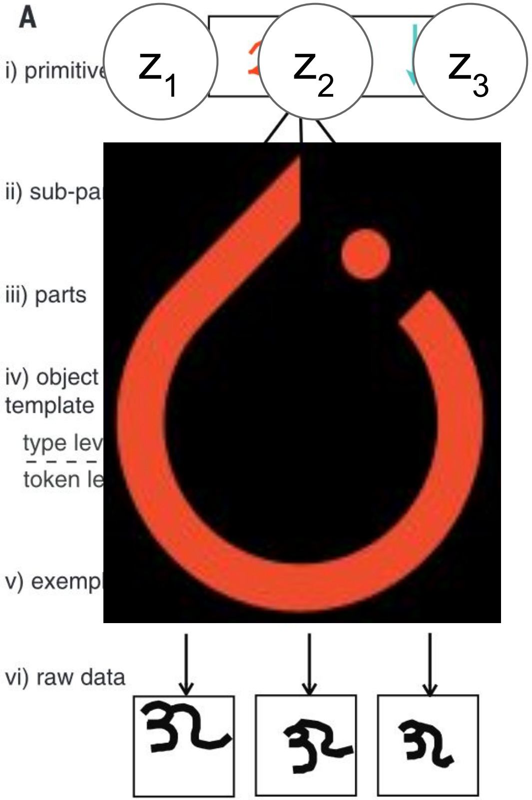
Decoder network: the simplest deep generative model



Model learning

We want to maximize the probability that a model *p(**x**, **z**)* generates data **x**:

$$\log p_\theta(x) = \log \int d\mathbf{z}\; p_\theta(\mathbf{x}, \mathbf{z})$$

But computing this integral directly is too difficult for most interesting models

Model learning and variational inference

Recall the definition of the ELBO from the previous tutorial:

$$\mathrm{ELBO} = C - \mathrm{KL}(q_\phi(\mathbf{z})||p(\mathbf{z}|x))$$

It turns out that the constant C is exactly the model log-evidence log p(x):

$$\mathrm{ELBO} = \log p_\theta(x) - \mathrm{KL}(q_\phi(\mathbf{z})||p_\theta(\mathbf{z}|x))$$

Model learning and variational inference

Recall that the KL divergence is non-negative.

Then the ELBO is a ***lower bound*** to the model's log ***evidence*** for any guide q***:***

$$\mathrm{ELBO} \leq \log p_\theta(x)$$

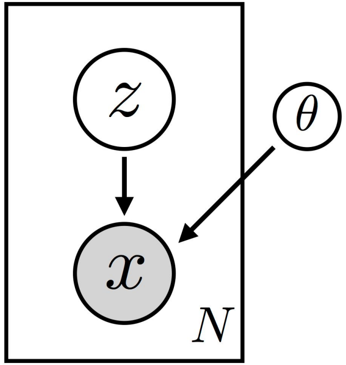
So we can learn a model by optimizing its parameters wrt the ELBO

Data: MNIST handwritten digits

Model

The decoder model samples a latent code, passes it through a neural network, and samples an observation:

```python
def model():
    pyro.module("decoder", nn_decoder)
    z = pyro.sample("z", Normal(0., 1.).expand_by([20]))
    bern_prob = nn_decoder(z)
    return pyro.sample("x", Bernoulli(bern_prob))
```



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

Model

The neural network `nn_decoder` is just a standard PyTorch `nn.Module`:

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

`pyro.module` just calls `pyro.param` on each of its parameters

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

Guide

The simplest guide: independent `Normal` distributions for each datapoint

```
def guide():
    ...
    loc_z = pyro.param("loc_z", ...)
    scale_z = pyro.param("scale_z", ...)
    return pyro.sample("z", Normal(loc_z, scale_z))
```

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Inference by optimization

Model learning could require learning a new guide for each model:

```
svi_guide = pyro.infer.SVI(model=conditioned_model_fixed_params, guide, ...)

svi_model = pyro.infer.SVI(model=conditioned_model, guide_fixed_params, ...)
```

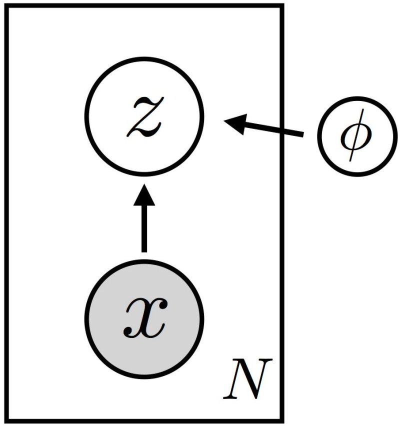
This is computationally infeasible with our mean-field guide:

```
for batch in batches:
    ...
    for t in range(100):
        svi_guide.step(batch)
    svi_model.step(batch)
```

Amortized guide

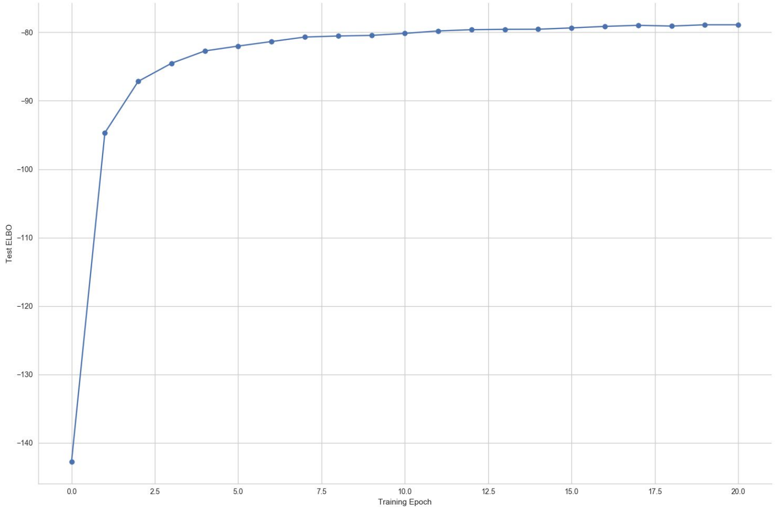
Instead of optimizing new parameters from scratch for each datapoint, we train a second neural network to guess the parameters of $q(\mathbf{z} \mid \mathbf{x})$:

```
def guide(x):
    pyro.module("encoder", encoder)
    loc_z, scale_z = encoder(x)
    return pyro.sample("z", dist.Normal(loc_z, scale_z))
```



VAE: inference

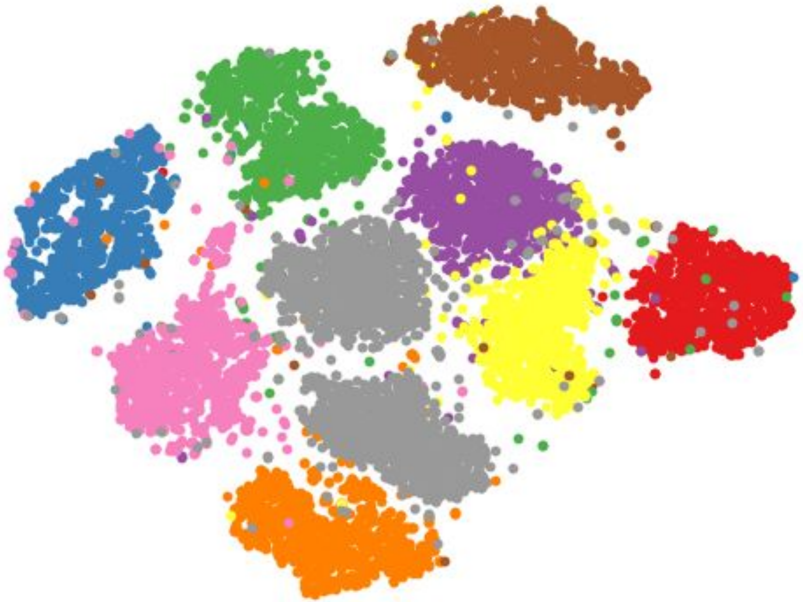
```
svi = pyro.infer.SVI(model=conditioned_model,
                     guide=guide,
                     optim=Adam({"lr": 0.001}),
                     loss=pyro.infer.Trace_ELBO())

for batch in batches:
    svi.step(batch)
```



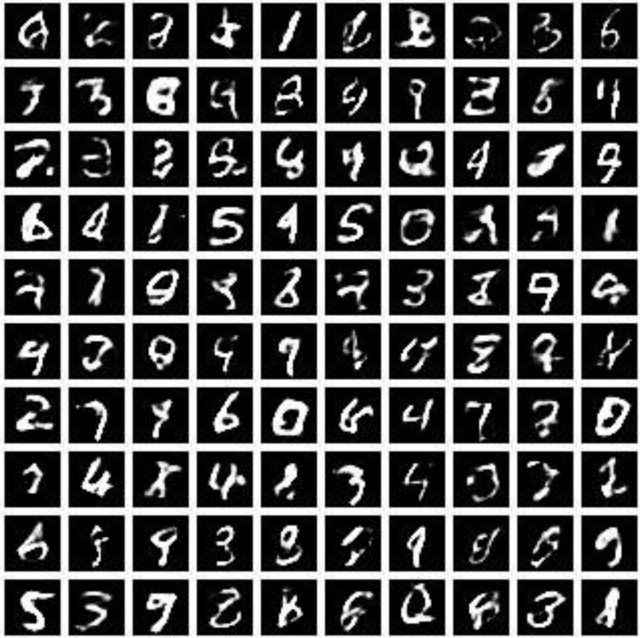
progress on elbo during training

VAE: results

latent embedding



samples from the generative model



[See our VAE tutorial for complete results]

Deep probabilistic programming on a postcard

```python
def model():
    pyro.module("decoder", decoder)
    z = pyro.sample("z", Normal(0., 1.).expand_by([20]))
    bern_prob = nn_decoder(z)
    return pyro.sample("x", Bernoulli(bern_prob))

def conditioned_model(x):
    return pyro.condition(model, data={"x": x})()


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

```python
def guide(x):
    pyro.module("encoder", nn_encoder)
    m_z, s_z = nn_encoder(x)
    return pyro.sample("z", dist.Normal(m_z, s_z))


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


for batch in batches:
    svi.step(batch)
```

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Estimating the ELBO

$$\mathrm{ELBO} \equiv \mathbb{E}_{q_\phi(\mathbf{z})}\left[\log p_\theta(\mathbf{x}, \mathbf{z}) - \log q_\phi(\mathbf{z})\right]$$

We keep using `pyro.infer.Trace_ELBO` for training guides:

```
svi = pyro.infer.SVI(..., loss=pyro.infer.Trace_ELBO())
```

Is this where all the complexity is hiding?

Poutine: building blocks for probabilistic programming

pyro.poutine: Composable higher-order functions (handlers) that compute side effects and modify behavior at sample and parameter sites

- **condition**: given a dict of sample site names and values, mark those sites as observed and set their outputs to the values in the dictionary
- **trace**: create a dictionary containing the inputs, functions, and outputs found at each sample and parameter site in a single execution
- **replay**: given a dictionary of sample sites and values, replace the output at each sample site with the value at that site in dictionary
- And others…

Internally, handlers install themselves on a global stack and pass messages up and down the stack at each sample and parameter site

Poutine: building blocks for probabilistic programming

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Estimating the ELBO

$$\text{ELBO} \equiv \mathbb{E}_{q_\phi(\mathbf{z})}\left[\log p_\theta(\mathbf{x},\mathbf{z}) - \log q_\phi(\mathbf{z})\right]$$

Pyro inference code can be as compact and readable as model code:

```
def simple_mc_elbo(model, guide, *args):
    guide_trace = trace(guide).get_trace(*args)
    model_trace = trace(replay(model, trace=guide_trace)).get_trace(*args)
    return model_trace.log_prob_sum() - guide_trace.log_prob_sum()
```

Estimating the ELBO

We add a negative sign, because PyTorch optimizers minimize:

```
def simple_mc_elbo(model, guide, *args):
    guide_trace = trace(guide).get_trace(*args)
    model_trace = trace(replay(model, trace=guide_trace)).get_trace(*args)
    elbo = model_trace.log_prob_sum() - guide_trace.log_prob_sum()
    return -elbo
```

This can now be used directly in place of `Trace_ELBO`:

```
svi = pyro.infer.SVI(..., loss=simple_mc_elbo)
```

Recap

1. Introduction to deep generative models and model learning
2. Implemented a simple deep generative model with Pyro
3. Performed variational inference with model learning in the VAE
4. Took a brief look at how Pyro works under the hood

Coming up: building up more complex models from the VAE

pyro.ai


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Would you like to know more?

Pyro tutorials web page: http://pyro.ai/examples/index.html

Detailed walkthrough of Pyro implementation of VAE:

http://pyro.ai/examples/vae.html

Deep dive into the math and implementation of stochastic variational inference in Pyro:

http://pyro.ai/examples/svi_part_i.html

Detailed description of tensor and distribution shapes and broadcasting in Pyro:

http://pyro.ai/examples/tensor_shapes.html