Probabilistic Programming and AI: Lecture 5

Advanced Topics in Probabilistic Programming

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Recap

- · Probabilistic programs can describe any probabilistic model
- Underlying models can be difficult to describe mathematically
 - · Unbounded number of random variables
 - Stochastic branching
 - · Dynamic distributions allowed (non-static support)
- · Efficient general-purpose inference is hard

Recap

- · General-purpose inference algorithms exist
 - importance sampling
 - · single-site MH
 - · Can be inefficient
- Imposing restrictions on the probabilistic program allows us to optimise inference
 - · fixed, finite number of continuous variables
 - · gradient-based inference: HMC, ADVI
 - · Still work for a large class of models

Outlook

- · We can optimise inference for individual models
- · Custom Inference: manually exploit structure of model
- · Data-Driven Inference: use observed data to improve proposals
- Probabilistic Programs as Proposals: convenient way to customise inference
- Deep Probabilistic Programming: learning proposals (and models) from data

Custom Inference

Infinite Mixture Models: Where single-site MH fails

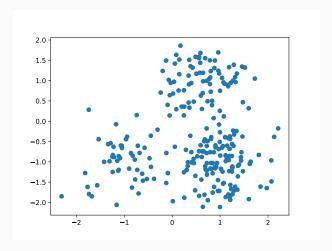
· Number of clusters:

$$K \sim Poisson(5)$$

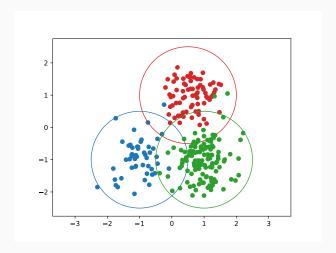
- Probability of being in cluster k, p_k : $p \sim \text{Dirichlet}(1/\text{K})$
- Cluster centers, k = 0, ..., K: $\mu_k^{\mathsf{X}} \sim \mathsf{Uniform}(\text{-3,3}),$ $\mu_k^{\mathsf{Y}} \sim \mathsf{Uniform}(\text{-3,3})$
- Cluster spread, $k=0,\ldots,K$: $\sigma_k^2 \sim \text{InverseGamma} \text{(1,1)}$
- Cluster membership, i = 1, ..., N: $z_i \sim \text{Categorical}(p)$
- Observed data, , i = 1, ..., N: $x_i \sim \text{Normal}(\mu_{z_i}, \sigma_{z_i})$

- Unbounded number of random variables
- · Discrete variables
- $\cdot \implies$ no HMC / ADVI
- High-dimensional
- $\cdot \implies$ no IS / LW
- but single-site MH is applicable in principle

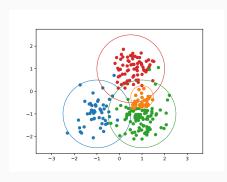
Data set



Ground truth



Single-site update



Updating the number of clusters *K*

- Adding clusters is easy: sample new cluster center and deviation
- How can we remove the orange cluster?
- Change K from 4 to 3 (single-site)
- Changes dimension of p (so current p has 0 log-prob?)
- Fix: sample p_k individually
- All memberships $z_i = 4$ have log-prob 0.

In theory, this update can happen, but is very low probability. All $z_i = 4$ have to be changed before setting K = 3.

In each iteration, we pick one type of move at random

- 1. Updating cluster centers μ_k and deviations σ_k
- 2. Reweighting clusters updating p
- 3. Updating the memberships z_i
- 4. Merging two randomly selected clusters.
- 5. Splitting one random cluster

Updating cluster centers μ_k and deviations σ_k

We can simply do random walk Metropolis Hastings updates.

Slightly perturbing the current values.

Reweighting clusters – updating p

Let n_k be the number of data points allocated to cluster k.

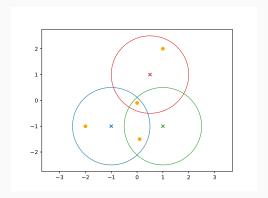
We expect that

$$\frac{n_k}{N} \approx p_k.$$

We can update *p* reflecting this relationship:

$$p \sim \text{Dirichlet}(n_1, \ldots, n_K)$$

Updating the memberships z_i



$$\tilde{w}_k := \mathcal{N}(x_i; \mu_k, \sigma_k) \propto \exp\left(-\frac{1}{2\sigma_k}(x_i - \mu_k)^\top (x_i - \mu_k)\right), \quad w_k := \frac{\tilde{w}_k}{\sum_{k=1}^K \tilde{w}_k}$$

$$z_i \sim \mathsf{Categorical}(w_1, \dots, w_k)$$

Merging two randomly selected clusters

Choose two "neighbouring" clusters with weights p_i , means μ_i and deviations σ_i at random, such that

$$\|\mu_1 - \mu_2\|_2 \le \|\mu_1 - \mu_j\|_2$$
, for $j = 1, ..., K$.

Match moments for isotropic Normals of dimension d:

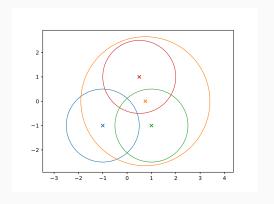
$$p_* = p_1 + p_2 (1)$$

$$p_*\mu_* = p_1\mu_1 + p_2\mu_2 \tag{2}$$

$$p_*(\mu_*^{\top}\mu_* + d\sigma_*^2) = p_1(\mu_1^{\top}\mu_1 + d\sigma_1^2) + p_2(\mu_2^{\top}\mu_2 + d\sigma_2^2)$$
 (3)

and update memberships z_i .

Merging two randomly selected clusters



Merge red and green cluster to orange.

Splitting one random cluster

Select cluster at random with weight p_* , mean μ_* and deviation σ_* .

Draw auxiliary variables:

$$u_1 \sim \text{Beta}(2,2)$$
, $u_2 \sim \text{Dirichlet}(2,\ldots,2) \in \mathbb{R}^d$, $u_3 \sim \text{Beta}(1,1)$

$$w_1 = w_* u_1, \tag{4}$$

$$w_2 = w_*(1 - u_1) (5)$$

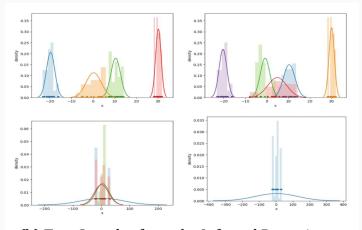
$$\mu_1 = \mu_* - u_2 \sigma_* \sqrt{d \frac{w_2}{w_1}} \tag{6}$$

$$\mu_2 = \mu_* + \mathbf{u}_2 \sigma_* \sqrt{d \frac{w_1}{w_2}} \tag{7}$$

$$\sigma_1 = u_3 (1 - u_2^{\mathsf{T}} u_2) \sigma_*^2 \frac{W_*}{W_1}$$
 (8)

$$\sigma_2 = (1 - u_3)(1 - u_2^{\top} u_2) \sigma_*^2 \frac{W_*}{W_2}$$
 (9)

These variables satisfy equations (1) - (3). Thus, merging the two randomly created clusters results in the original cluster (p_*, μ_*, σ_*) .



(b) Two Samples from the Inferred Posterior: Richardson & Green's Data-driven MCMC (top), BLOG Ancestral Sampling (bottom)

- In the proposal, we make use of auxiliary random variables
- · This makes computing the acceptance probability non-trivial
- It is key to be able to "undo" moves, e.g. merge join
- This is called reversible-jump MCMC
- It is a special case of involutive MCMC
- More details in: On Bayesian Analysis of Mixtures with an Unknown Number of Components (with discussion) https://academic.oup.com/jrsssb/article-pdf/59/ 4/731/49588858/jrsssb_59_4_731.pdf

Data-Driven Proposals = Biased Inference?

- It is often good practice to chose *uninformative* priors, i.e. we do not prefer any values for the latent variables *a-priori*
- However, with the proposals, we want to stir inference towards high probability areas of the posterior
- We can use the observed data to construct proposals as close to the posterior as possible

Data-Driven Proposals

However, to ensure convergence to the true posterior proposals have to satisfy following properties:

- Unconditional proposals Q(x): if a state x is possible according to the model P(x) > 0, then it has to be possible according to the proposal Q(x) > 0
- Conditional proposals Q(x'|x): any state should be reachable from any other state in any number of steps less or equal to a fixed number N.

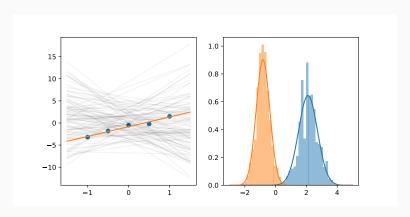
Common strategy:

One way of constructing data-driven proposals is to use a **heuristic to estimate the mode** of the target distribution (or one of its conditional distributions) and to sample values near the estimate of the mode, but with **noise added**.

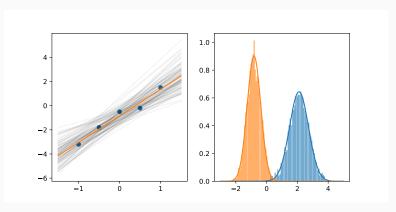
With enough data:

mode of posterior ≈ maximum likelihood estimator

Linear regression: propose from prior

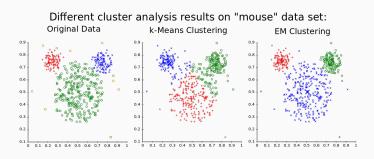


Linear regression: propose from Normals centered at ordinary least squares (OLS) solution



GMM:

Sample number of clusters $K \sim \text{Poisson(5)}$ Run k-means clustering and perturb the result.



Probabilistic Programs as Proposals

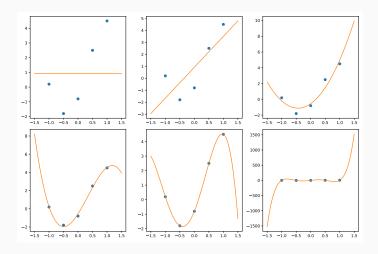
Probabilistic Programs as Proposals

As proposals get more complex it is more convenient to write them programmatically.

Key idea: We can write a probabilistic program and use it for generating proposal in the inference for another program.

These programs are called guides.

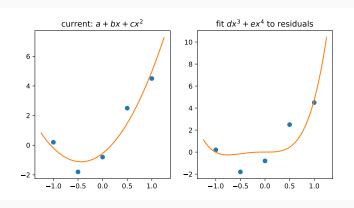
Gen (and Pyro): programmable inference



```
@gen function poly model(x coordinates)
    degree ~ uniform_discrete(0,4)
    var ~ inv_gamma(1,1)
    coefficients = [(\{(:c,i)\} \sim normal(0,1)) \text{ for } i \text{ in } 0:degree]
    for i = 1:length(x_coordinates)
        x = x_coordinates[i]
        mu = 'coefficients * x.^(0:degree)
         {(:y,i)} ~ normal(mu, sqrt(var))
    end
end
@gen function poly proposal prior(x coordinates)
    degree ~ uniform_discrete(0,4)
    var ~ inv_gamma(1,1)
    coefficients = [(\{(:c,i)\} \sim normal(0,1))] for i in 0:degree]
end
```

Idea: Iteratively sampling coefficients.

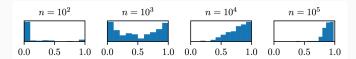
We have currently polynomial of 2nd degree.



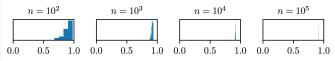
Sample value centered around OLS solution for d.

```
@gen function poly_proposal_data_driven(x_coords, y_coords)
    # noise for each coefficient
    scales = [0.395, 0.242, 0.088, 0.020, 0.007]
    n = length(x_coords)
    degree ~ uniform_discrete(0,4)
    coeffs = [NaN for i in 0:degree]
    predicted = zeros(n)
    for i in 0:degree
        residuals = y_coords .- predicted # elementwise subtraction
        # fit a polynomial to residuals with coefficients 0..i-1 fixed to zero
        est coeffs = least squares(x coords, residuals, degree, min degree=i)
        coeffs[i+1] = (\{(:c,i)\} \sim cauchy(est coeffs[1], scales[i+1]))
        predicted = [dot(coeffs, x.^{(0:i)}) for x in x coords]
    end
    # use variance of residuals to get estimate for model noise
    residuals = v coords .- predicted
    var \sim inv gamma(1 + n/2, 1 + 0.5 * dot(residuals, residuals))
end
```

Estimate for the probability of degree = 3



(a) Estimates from self-normalized importance sampling with a prior proposal.



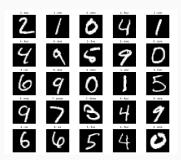
(b) Estimates from self-normalized importance sampling with a data-driven proposal.

Deep Probabilistic Programming

Deep Probabilistic Programming: Motivation

- Non-programmability: For many data modalities that are commonly considered in ML and AI, including images and natural language, it is near-impossible to fully specify a probabilistic program that defines a sufficiently realistic distribution over data.
- Scalability: Models in ML and AI are routinely trained on very large datasets. Most inference methods that we have considered so far do not scale to such large datasets without additional modifications.
- These challenges can be addressed by combining inference methods from probabilistic programming with differentiable programming techniques from deep learning research.

Deep Probabilistic Programming: Non-programmability



Non-programmability:

How to implement a probabilistic program that generates 28×28 px images of hand-written digits?

Sample digit \sim DiscreteUniform(0, 9),

and then ??

Deep Probabilistic Programming: Neural Networks

- · Neural networks are universal function approximators
- Use neural network η_{λ} with parameters λ in the program to flexibly model relationship between latents and observes
- · latent: digit; observed: image
- · image[x,y] \sim Bernoulli($\eta_{\lambda}(\text{digit})[x,y]$)
- \cdot probability of pixel being white \cong gray scale value
- Learn λ to fit our data set

Deep Probabilistic Programming: Neural Networks

How to learn λ (model parameters)?

• Fully Bayesian treatment: λ are additional latent variables, set prior $P(\lambda)$ and take maximum a-posteriori (MAP)

$$\operatorname{argmax}_{\lambda} P(\lambda | X_1, \dots, X_n)$$
?

- $\cdot
 ightarrow$ Bayesian deep learning
- · Challenges: very high-dimensional posterior + choice of prior
- Instead maximise marginal likelihood of training data $\operatorname{argmax}_{\lambda} P(x_1, \dots, x_n | \lambda)$
- $\cdot \rightarrow$ Maximum likelihood estimation (MLE)
- $P(\lambda|X_1,\ldots,X_n) \propto P(X_1,\ldots,X_n|\lambda)P(\lambda)$
- When there is a lot of data, the likelihood $P(X|\lambda)$ numerically dominates the prior $P(\lambda)$ so effectively the prior can be ignored (formally: Bernstein von Mises theorem)
- · MLE \approx MAP if we have a lot of data

Find MLE of λ with stochastic gradient ascent

$$\nabla_{\lambda} \log P(X|\lambda) = \mathbb{E}_{\theta \sim P(.|X,\lambda)} \left[\nabla_{\lambda} \log P(X,\theta|\lambda) \right]$$

because

$$\mathbb{E}_{\theta \sim P(.|X,\lambda)} \left[\nabla_{\lambda} \log P(X,\theta|\lambda) \right]$$

$$= \mathbb{E}_{\theta \sim P(.|X,\lambda)} \left[\nabla_{\lambda} \log P(X|\lambda) + \nabla_{\lambda} \log P(\theta|X,\lambda) \right]$$

$$= \nabla_{\lambda} \log P(X|\lambda) + \underbrace{\mathbb{E}_{\theta \sim P(.|X,\lambda)} \left[\nabla_{\lambda} \log P(\theta|X,\lambda) \right]}_{=0}$$

How to compute $\mathbb{E}_{\theta \sim P(.|X,\lambda)} [\nabla_{\lambda} \log P(X,\theta|\lambda)]$?

Bayesian inference!

- · We do not only want to learn the model parameters
- We also want to perform posterior inference over latent variables
- E.g. what is the digit of an unlabeled image?
- · How to combine model learning and posterior inference?

Variational guide programs

- If we cannot fully specify the model, then we probably also want to specify the proposals with neural networks η_{ϕ} .
- · E.g. mapping images to their digit.
- Thus, we write a variational proposal distribution as a guide program.
- As in ADVI, we can differentiate through the neural networks and maximise the ELBO to minimise the KL-divergence.

Scalability: Amortised Inference

Instead of learning N variational distributions separately like in ADVI with mean-field approximation,

$$Q(\theta_i|x_i,\phi)=Q(\theta_i|\phi_i),$$

we use the neural network η_{ϕ} to predict the variational parameters for each observation x_i ,

$$Q(\theta_i|X_i,\phi)=Q(\theta_i|\eta_\phi(X_i)).$$

E.g. for N images of hand-written digits x_i :

Learning N separate distributions over the true latent digits θ_i of x_i versus learning to predict the digit of each image $\eta_{\phi}(x_i)$ and then build a distribution around it.

Combining model learning and posterior inference

· Maximising the ELBO w.r.t to ϕ and λ

$$\begin{split} \mathsf{ELBO}(X;\lambda,\phi) &= & \mathbb{E}_{\theta \sim \mathcal{Q}(.|\phi)} \left[\log P(\theta,X|\lambda) - \log \mathcal{Q}(\theta|\phi) \right] \\ &= & \log P(X|\lambda) - D_{\mathsf{KL}} (\mathcal{Q}(\Theta|\phi) \parallel P(\Theta|X,\lambda)) \end{split}$$

• Justification: assume we have variational distribution with an "infinity capacity" (it can fit every distribution perfectly), then

$$\min_{\phi} D_{\mathsf{KL}}(Q(\Theta|\phi) \parallel P(\Theta|X,\lambda)) = 0 \text{ and } \max_{\phi} \mathsf{ELBO}(X;\lambda,\phi) = \log P(X|\lambda)$$

• Thus, maximising the ELBO w.r.t to ϕ and λ is equivalent to maximum likelihood estimation,

$$\max_{\lambda} \max_{\phi} \mathsf{ELBO}(X; \lambda, \phi) = \max_{\lambda} \log P(X|\lambda)$$

Maximising the ELBO w.r.t to ϕ and λ

$$\max_{\lambda} \max_{\phi} \mathsf{ELBO} \big(\mathsf{X}; \lambda, \phi \big) = \max_{\lambda} \log P \big(\mathsf{X} | \lambda \big)$$

- In practice, we will not have an infinite capacity variational distribution, and we will typically not fully solve the inner optimization problem for ϕ at every gradient step for λ .
- We take gradient steps in both λ and ϕ space simultaneously so that the guide and model play chase, with the guide tracking a moving posterior $\log P(\Theta|X,\lambda)$.
- There will be a difference between maximizing the ELBO and maximizing the marginal likelihood. This difference manifests itself as an extra term in the gradient

$$\nabla_{\lambda} ELBO(X; \lambda, \phi) = \nabla_{\lambda} \log P(X|\lambda) + \nabla_{\lambda} D_{KL}(Q(\Theta|\phi) \parallel P(\Theta|X, \lambda))$$

Maximising the ELBO w.r.t to ϕ and λ

$$\nabla_{\lambda} \mathsf{ELBO} \big(\mathsf{X}; \lambda, \phi \big) = \nabla_{\lambda} \log P \big(\mathsf{X} | \lambda \big) + \nabla_{\lambda} D_{\mathsf{KL}} \big(Q \big(\Theta | \phi \big) \parallel P \big(\Theta | \mathsf{X}, \lambda \big) \big)$$

In this gradient, the second term prevents gradient updates to λ from making changes to the model that strongly increase the KL relative to the variational approximation. This is sometimes argued to be beneficial, in the sense that it acts as a form of regularization that prevents overfitting in the generative model, or in the sense that it stabilizes the optimizer. However, it can also lead to approximation errors in the learned generative model.

Optimizing the ELBO will balance maximizing $\log P(X|\lambda)$ against minimizing $D_{\text{KL}}(Q(\Theta|\phi) \parallel P(\Theta|X,\lambda))$. This can be seen as a bias towards learned $P(\Theta|X,\lambda)$ that are "compatible" with performing variational inference in using the variational family $Q(\Theta|\phi)$.

Maximising the ELBO w.r.t to ϕ and λ - Computing Gradients

As

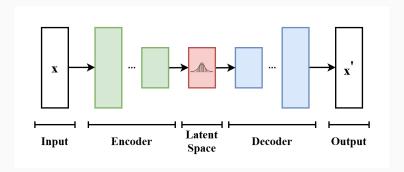
$$\mathsf{ELBO}(X; \lambda, \phi) = \mathbb{E}_{\theta \sim Q(.|\phi)} [\log P(X, \theta | \lambda) - \log Q(\theta | \phi)]$$

is an expectation w.r.t to $Q(.|\phi)$, we can pull ∇_{ϕ} inside the expectation if we can apply the reparametrisation trick as in ADVI. This allows us to use unbiased lower-variance Monte-Carlo estimates for the gradient.

 ∇_{λ} can always be pulled inside the expectation.

Deep Probabilistic Programming - Example

Semi-Supervised Variational Auto-Encoders (SSVAE) in Pyro



Objective: Learn generative distribution of hand-written digits and be able to predict the digit of unlabeled images.

Only a fraction of the images are assumed to be labeled.

```
# observation likelihood p(x|z)
class Decoder(nn.Module):
    def __init__(self, input_dim, output_dim, hidden dims):
        super(). __init__()
        self.fc1 = nn.Linear(input dim, hidden dims[0])
        self.fc2 = nn.Linear(hidden dims[0], hidden dims[1])
        self.fc3 = nn.Linear(hidden dims[1], output dim)
        self.softplus = nn.Softplus()
    def forward(self, z):
        z = self.softplus(self.fc1(z))
        z = self.softplus(self.fc2(z))
        loc img = torch.sigmoid(self.fc3(z))
        return loc img # probabilities of pixels being white
```

```
def model(self, x, y=None):
    pyro.module("decoder", self.decoder)
   with pyro.plate("data", x.shape[0]):
        # setup hyperparameters for prior p(z)
        z loc = torch.zeros(x.shape[0], self.z dim)
        z_scale = torch.ones(x.shape[0], self.z_dim)
        \# sample from prior p(z)
        z = pyro.sample("latent", dist.Normal(z_loc, z_scale).to_event(1))
        # setup hyperparameters for prior p(y)
        alpha = torch.full(x.shape[0], 1/self.output_size)
        # sample from prior p(y)
        y = pyro.sample("y", dist.OneHotCategorical(alpha), obs=y)
        # sample from p(x|y,z)
        loc_img = self.decoder.forward(self.concat.forward(z, y))
        # sample image
        pyro.sample(
            "obs".
            dist.Bernoulli(loc_img, validate_args=False).to_event(1),
            obs=x.
        return loc_img
```

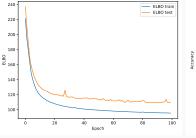
```
# diagonal gaussian distribution q(z|x,y)
class EncoderZ(nn.Module):
    def __init__(self, input_dim, output_dim, hidden_dims):
        super(). init ()
        self.input dim = input dim
        self.fc1 = nn.Linear(input dim. hidden dims[1])
        self.fc2 = nn.Linear(hidden dims[1], hidden dims[0])
        # two heads for mean and std
        self.fc31 = nn.Linear(hidden_dims[0], output_dim)
        self.fc32 = nn.Linear(hidden dims[0]. output dim)
        self.softplus = nn.Softplus()
    def forward(self. x):
        x = self.softplus(self.fc1(x))
        x = self.softplus(self.fc2(x))
        z loc = self.fc31(x)
        z_scale = torch.exp(self.fc32(x))
        return z loc, z scale
```

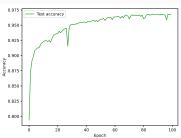
```
# diagonal gaussian distribution q(y|x)
class EncoderY(nn.Module):
    def __init__(self, input_dim, output_dim, hidden_dims):
        super(). init ()
        self.input dim = input dim
        self.fc1 = nn.Linear(input dim, hidden dims[1])
        self.fc2 = nn.Linear(hidden dims[1], hidden dims[0])
        self.fc3 = nn.Linear(hidden dims[0], output dim)
        self.softplus = nn.Softplus()
        self.softmax = nn.Softmax(dim=1)
    def forward(self. x):
        x = self.softplus(self.fc1(x))
        x = self.softplus(self.fc2(x))
        v = self.softmax(self.fc3(x)) # returns class probabilities
        return v
```

```
# define the guide (variational distribution) q(z|x,y) q(y|x)
def guide(self, x, y=None):
    pyro.module("encoder z", self.encoder z)
    pyro.module("encoder_y", self.encoder_y)
    with pyro.plate("data", x.shape[0]):
        if v is None:
            # use the encoder to get the parameters used to define q(y|x)
            alpha = self.encoder_y.forward(x)
            # sample q(v|x)
            v = pvro.sample("v". dist.OneHotCategorical(alpha))
        # amortised inference
        # use the encoder to get the parameters used to define q(z|x,v)
        z_loc, z_scale = self.encoder_z.forward(self.concat.forward(x, y))
        # sample q(z|x,y)
        z = pyro.sample("latent", dist.Normal(z_loc, z_scale).to_event(1))
```

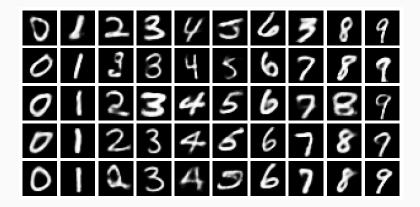
```
for epoch in range(1, epochs+1):
    # perform svi steps on train loader
   epoch loss = 0.0
   # batches are not shuffled
   for i, (x, y) in enumerate(loaders['train']):
        x = x.reshape(-1, ssvae.input_size).to(device)
        # alternate between supervised and unsupervised batches
        if nth supervised and (i % nth supervised == 0):
            y = F.one_hot(y, ssvae.output_size).to(device)
            # perform step on auxiliary model
            if aux loss:
                epoch loss += svi aux.step(x. v)
        else.
            v = None
        epoch_loss += svi.step(x, y)
```

ELBO + classification accuracy for data set with 10% labeled





Newly generated digits



Resources

```
Probabilistic Graphical Models - D Koller, N Friedman - 2009:
Chapter 2.1.4 and 3
```

Paper: On Bayesian Analysis of Mixtures with an Unknown Number of Components (with discussion)

https://academic.oup.com/jrsssb/article-pdf/59/4/731/49588858/jrsssb_59_4_731.pdf

RJMCMC / Involutive MCMC in Gen Tutorial https://www.gen.dev/tutorials/rj/tutorial

Paper: Transforming Worlds: Automated Involutive MCMC for Open-Universe Probabilistic Models https://people.eecs.berkeley.edu/~russell/papers/aabi21-oupm.pdf

Data-Driven Proposals in Gen Tutorial https://www.gen.dev/tutorials/data-driven-proposals/tutorial

Resources

Paper: Using probabilistic programs as proposals https://arxiv.org/pdf/1801.03612.pdf

Paper: Pyro: Deep Universal Probabilistic Programming

https://arxiv.org/pdf/1810.09538.pdf

An Introduction to Probabilistic Programming: Chapter 8 Deep

Probabilistic Programming

https://arxiv.org/pdf/1809.10756.pdf

Pyro ELBO Gradients Estimators

https://pyro.ai/examples/svi_part_iii.html

Paper: Auto-Encoding Variational Bayes

https://arxiv.org/pdf/1312.6114.pdf

Pyro Semi-Supervised Variational Auto-Encoder

https://pyro.ai/examples/ss-vae.html

Organisation

- · Today was last lecture
- · 29.11. A4 Deadline
- · 04.12. Assignment Discussion Session
- · 06.12. Project Proposal Deadline
- 08.01. Project Milestone
- · 28.01. & 29.01. Project Presentations