VAE with Discrete Variables For Semi-Supervised Learning

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Presentation: Nadezhda Chirkova

VAE: reminder

Model for one image:

Training data

$$p(x, z \mid \theta) = p(z)p(x \mid z, \theta)$$

$$p(z) = \mathcal{N}(z \mid 0, I)$$ ⟵ Prior over latent code

$$p(x \mid z, \theta) = \prod_{i=1}^{D} p_i(z, \theta)^{x_i} (1 - p_i(z, \theta))^{1 - x_i}.$$ ⟵ Likelihood of data (here — Bernoulli distribution)

neural network

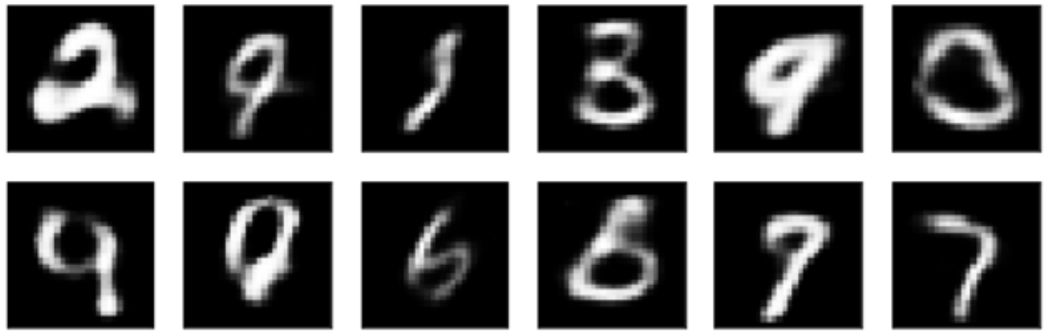
x - data (binary image) z - latent code (continuous d-dim vector)

VAE as a generative model (“testing” stage)

Generate a new image:

$$1.\ z \sim p(z)$$

$$2.\ x \sim p(x|z,\theta)$$



Generated images

1. $z \rightarrow NN \rightarrow \{\log p_i(z,\theta)\}_{i=1,\ldots,D}$
2. Sample $x_i = 0/1,\ i = 1,\ldots,D$

or use probabilities as pixels

VAE as a generative model (“testing” stage)

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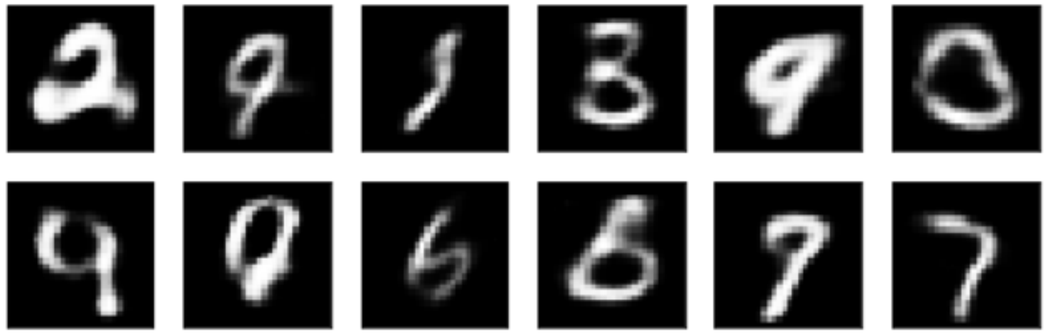

Generated images

θ?

1. $z \rightarrow NN \rightarrow \{\log p_i(z,\theta)\}_{i=1,\ldots,D}$
2. Sample $x_i = 0/1,\ i = 1,\ldots,D$

or use probabilities as pixels

Training VAE

$$\log p(x|\theta) \geqslant \mathbb{E}_{q(z|x)} \log p(x|z,\theta) - KL(q(z|x)||p(z)) + KL(q(z|x)||p(z|x)) \quad \forall q$$

does not depend on q

max

$\Leftrightarrow$

min

$$q(z|x,\phi) \approx p(z|x) \leftrightarrow$$

$$\mathcal{L}(\theta,\phi) = \sum_{n=1}^{N} \mathbb{E}_{q(z_n|x_n,\phi)} \log p(x_n|z_n,\theta) - KL(q(z_n|x_n,\phi)||p(z_n)) \to \max_{\theta,\phi}$$

Training VAE

$$\log p(x|\theta) \geqslant \mathbb{E}_{q(z|x)} \log p(x|z,\theta) - KL(q(z|x)||p(z)) + KL(q(z|x)||p(z|x)) \quad \forall q$$

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$$q(z|x,\phi)?$$

Training VAE

$$q(z \mid x, \phi) = \mathcal{N}(z \mid \mu(x, \phi), \mathrm{diag}(\sigma^2(x, \phi)))$$

neural network

Training VAE

$$q(z \mid x, \phi) = \mathcal{N}(z \mid \mu(x, \phi), \text{diag}(\sigma^2(x, \phi)))$$

$$\mathcal{L}(\theta, \phi) = \sum_{n=1}^{N} \mathbb{E}_{q(z_n|x_n,\phi)} \log p(x_n|z_n, \theta) - KL(q(z_n|x_n, \phi)||p(z_n)) \to \max_{\theta,\phi}$$

$$\mathcal{L}(\theta, \phi) = \sum_{n} \mathbb{E}_{q(z_n|x_n,\phi)} [\log p(x_n|z_n, \theta) + \log p(z_n) - \log q(z_n|x_n, \phi)] \to \max_{\theta,\phi}$$

?

Bernoulli pdf

Gaussian pdf

Gaussian pdf

Training VAE

$$q(z \mid x, \phi) = \mathcal{N}(z \mid \mu(x, \phi), \operatorname{diag}(\sigma^2(x, \phi)))$$

$$\mathcal{L}(\theta, \phi) = \sum_{n=1}^{N} \mathbb{E}_{q(z_n|x_n,\phi)} \log p(x_n|z_n, \theta) - KL(q(z_n|x_n, \phi)||p(z_n)) \to \max_{\theta,\phi}$$

$$\mathcal{L}(\theta, \phi) = \sum_{n} \mathbb{E}_{q(z_n|x_n,\phi)} [\log p(x_n|z_n, \theta) + \log p(z_n) - \log q(z_n|x_n, \phi)] \to \max_{\theta,\phi}$$

?

Bernoulli pdf

Gaussian pdf

Gaussian pdf

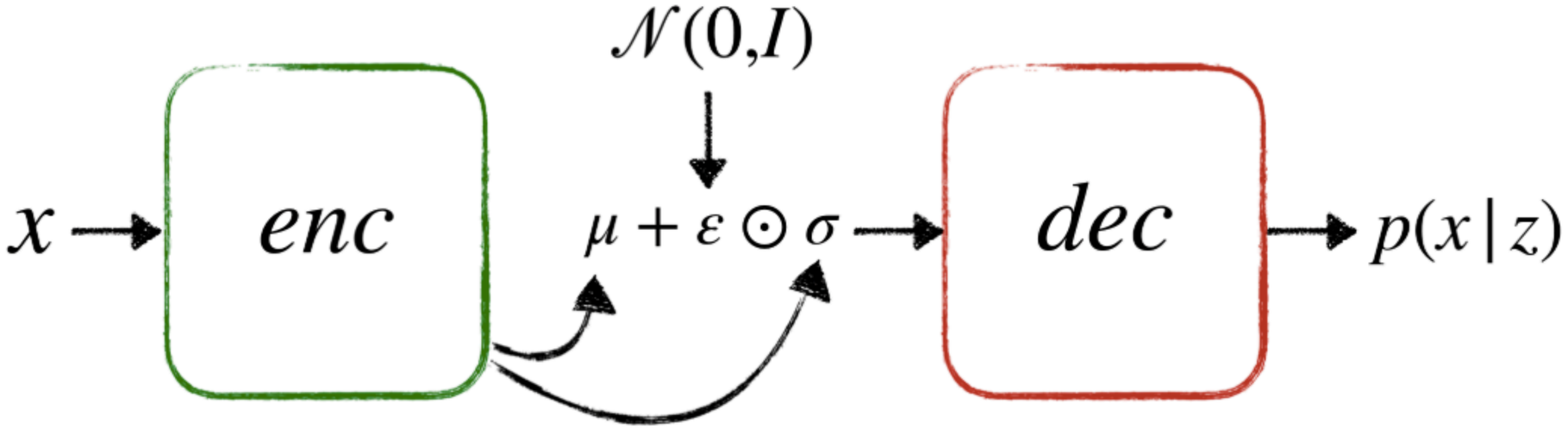
Sample mini-batch + Monte-Carlo sample + Reparametrization trick:

$$\mathbb{E}[\dots] \approx \log p(x|z_0, \theta) + \log p(z_0) - \log q(z_0|x, \phi)$$

$$z_0 = \mu(x, \phi) + \sigma(x, \phi) \odot \varepsilon_0$$

$$\varepsilon_0 \sim \mathcal{N}(0, I)$$

VAE: computational graph

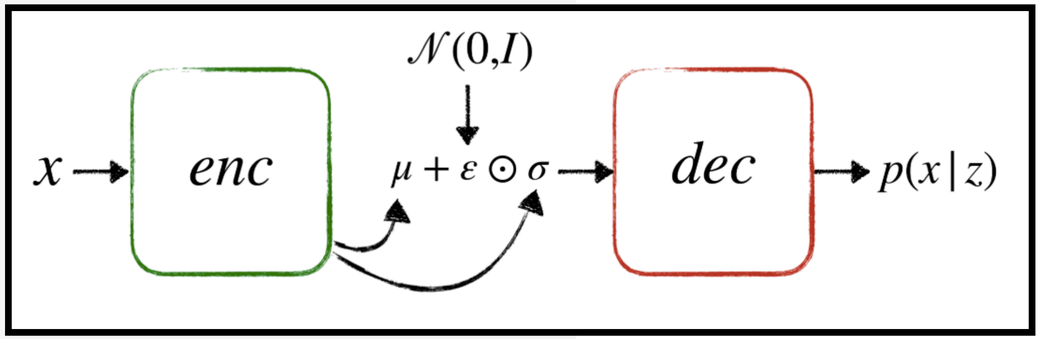


VAE: code: defining encoder and decoder

```
d, nh, D = 32, 100, 28 * 28

enc = nn.Sequential(
    nn.Linear(D, nh),
    nn.ReLU(),
    nn.Linear(nh, nh),
    nn.ReLU(),
    nn.Linear(nh, 2 * d))

dec = nn.Sequential(
    nn.Linear(d, nh),
    nn.ReLU(),
    nn.Linear(nh, nh),
    nn.ReLU(),
    nn.Linear(nh, D)).to(device)

enc = enc.to(device)
dec = dec.to(device)
```

VAE: code: computing loss

```
def loss_vae(x, encoder, decoder):
    """
    returns
    1. the avergave value of negative
       ELBO across the minibatch x
    2. and the output of the decoder
    """
    batch_size = x.size(0)
    encoder_output = encoder(x)
    pz = Independent(Normal(loc=torch.zeros(batch_size, d).to(device),
                            scale=torch.ones(batch_size, d).to(device)),
                     reinterpreted_batch_ndims=1)
    qz_x = Independent(Normal(loc=encoder_output[:, :d],
                              scale=torch.exp(encoder_output[:, d:])),
                       reinterpreted_batch_ndims=1)

    z = qz_x.rsample() # reparametrization inside!
    decoder_output = decoder(z)
    px_z = Independent(Bernoulli(logits=decoder_output),
                       reinterpreted_batch_ndims=1)
    loss = -(px_z.log_prob(x) + pz.log_prob(z) - qz_x.log_prob(z)).mean()
    return loss, decoder_output
```



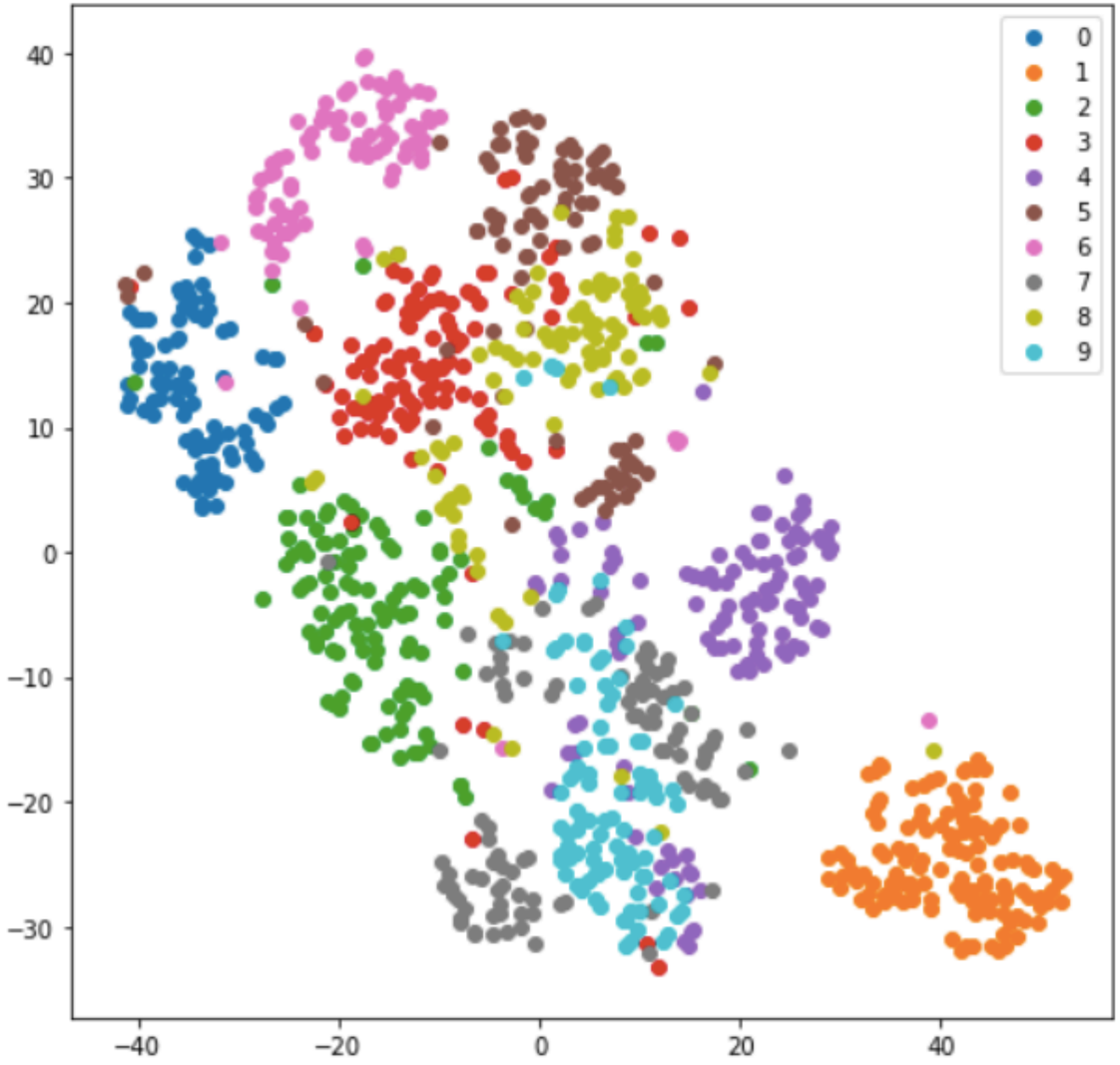
torch.distributions used to:

1) compute pdf
2) sample

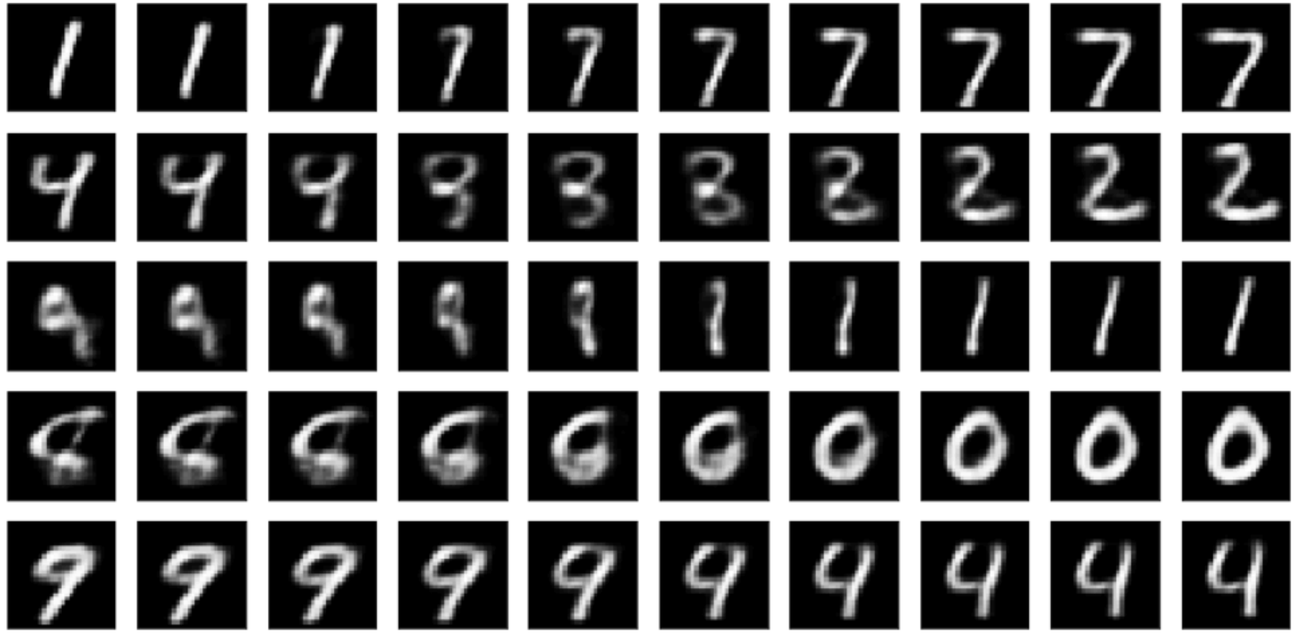
```
from torch.distributions
import Normal,
       Bernoulli,
       Independent
```

VAE: visualization

tSNE of the latent code mean values



interpolation in the latent space



VAE for semi-supervised learning

Semi-supervised Learning with Deep Generative Models

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CATEGORICAL REPARAMETERIZATION WITH GUMBEL-SOFTMAX

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VAE for semi-supervised learning

Semi-supervised learning: classification when only a small subset of the observations have corresponding class labels.

VAE for semi-supervised learning: model labels along with latent codes.

VAE for semi-supervised learning

Model for one image:

$$p(x, y, z) = p(x \mid y, z)p(z)p(y)$$

$$p(y) = Cat(y \mid \pi_0), \pi_0 = (1/10, \ldots, 1/10)$$

$$p(z) = \mathcal{N}(z \mid 0, I)$$

Priors over class label and latent code

$$p(x \mid y, z) = \prod_{i=1}^{D} p_i(y, z)^{x_i} (1 - p_i(y, z))^{1-x_i}$$

Likelihood of data (Bernoulli distribution)

neural network

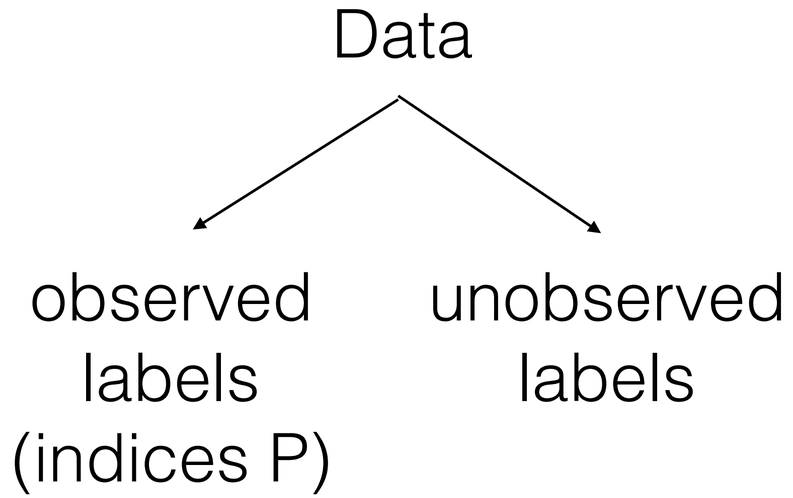
* We now drop parameters in conditioning since formulas are already very impressive

SS-VAE as a generative model

Generate a new image:

1. $z \sim p(z)$
2. $y \sim p(y)$
3. $x \sim p(x|y,z)$

Training SS-VAE



$$LogLikelihood(X, y) = \sum_{i \notin P} \log p(x_i) + \sum_{i \in P} \log p(x_i, y_i)$$

Training SS-VAE

$$LogLikelihood(X, y) = \sum_{i \notin P} \log p(x_i) + \sum_{i \in P} \log p(x_i, y_i)$$

For observed labels (similar to VAE):

$$q(z \mid y, x) = \mathcal{N}(z \mid \mu_\phi(x, y), \operatorname{diag} \sigma^2_\phi(y, x))$$

$$\log p(x, y) = \log \mathbb{E}_{p(z)} p(x, y \mid z) \geq$$

$$\mathbb{E}_{q(z|y,x)} \log \frac{p(x, y \mid z) p(z)}{q(z \mid y, x)}$$

Training SS-VAE

$$LogLikelihood(X, y) = \sum_{i \notin P} \log p(x_i) + \sum_{i \in P} \log p(x_i, y_i)$$

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$$\mathbb{E}_{q(z|y,x)} \log \frac{p(x, y \mid z) p(z)}{q(z \mid y, x)}$$

For unobserved labels:

$$q(y, z \mid x) = q(y \mid x) q(z \mid y, x)$$

$$q(y \mid x) = Cat(y \mid \pi(x))$$

$$q(z \mid y, x) = \mathcal{N}(z \mid \mu_\phi(x, y), \operatorname{diag} \sigma^2_\phi(y, x))$$

$$\log p(x) = \log \mathbb{E}_{p(y)} \mathbb{E}_{p(z|y)} \log p(x \mid z, y) \geq$$

$$\mathbb{E}_{q(y|x)} \mathbb{E}_{q(z|y,x)} \log \frac{p(x \mid y, z) p(y) p(z)}{q(z \mid y, x) q(y \mid x)}$$

Training SS-VAE

Final objective:

$$\mathcal{L}(X, y) = \sum_{i \in P} \mathbb{E}_{q(z_i|y_i,x_i)} \log \frac{p(x_i, y_i \mid z_i)p(z_i)}{q(z_i \mid y_i, x_i)} + \sum_{i \notin P} \mathbb{E}_{q(y_i|x_i)} \mathbb{E}_{q(z_i|y_i,x_i)} \log \frac{p(x_i \mid y_i, z_i)p(y_i)p(z_i)}{q(z_i \mid y_i, x_i)q(y_i \mid x_i)}$$

sample from Gaussian distr: reparam. trick

known pdfs

sample from categorical distr.: **?**

sample from Gaussian distr: reparam. trick

known pdfs

Training SS-VAE

Final objective:

$$\mathcal{L}(X, y) = \sum_{i \in P} \mathbb{E}_{q(z_i|y_i,x_i)} \log \frac{p(x_i, y_i \mid z_i)p(z_i)}{q(z_i \mid y_i, x_i)} + \sum_{i \notin P} \mathbb{E}_{q(y_i|x_i)} \mathbb{E}_{q(z_i|y_i,x_i)} \log \frac{p(x_i, y_i \mid z_i)p(z_i)}{q(z_i \mid y_i, x_i)q(y_i \mid x_i)}$$

- $\mathbb{E}_{q(z_i|y_i,x_i)}$: sample from Gaussian distr: reparam. trick
- $\frac{p(x_i, y_i \mid z_i)p(z_i)}{q(z_i \mid y_i, x_i)}$: known pdfs
- $\mathbb{E}_{q(y_i|x_i)}$: sample from categorical distr.: **Gumbel-Softmax trick**
  - without trick: |Y| forward passes
  - with trick: 1 forward pass
- $\mathbb{E}_{q(z_i|y_i,x_i)}$: sample from Gaussian distr: reparam. trick
- $\frac{p(x_i, y_i \mid z_i)p(z_i)}{q(z_i \mid y_i, x_i)q(y_i \mid x_i)}$: known pdfs

Training SS-VAE: important practical aspect

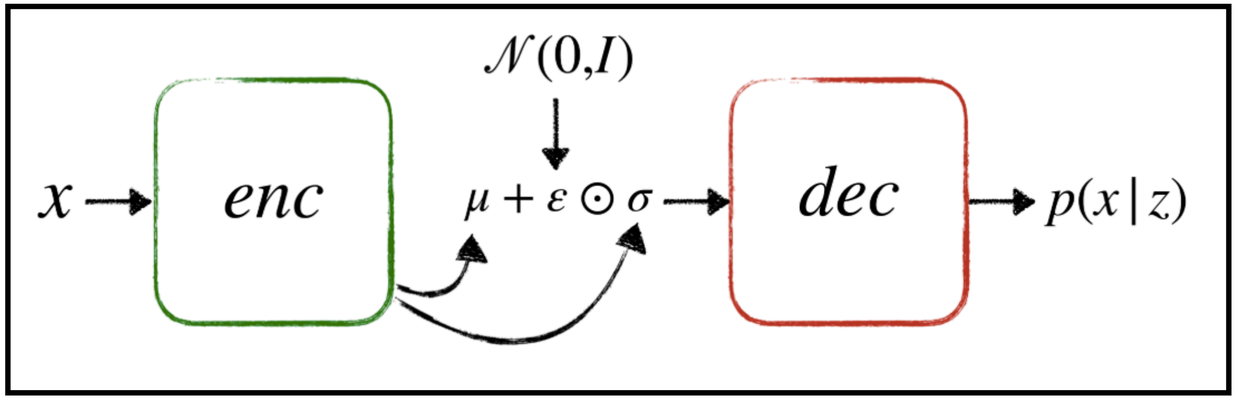
ELBO maximization does not lead to any semantics in latent variables y.

We are going to restrict variational approximations $q(y \mid x)$ to the ones that correctly classify observation x on fully-observed variables (x_i, y_i). As in the original paper, we will add a cross-entropy regularizer to the objective with weight α:

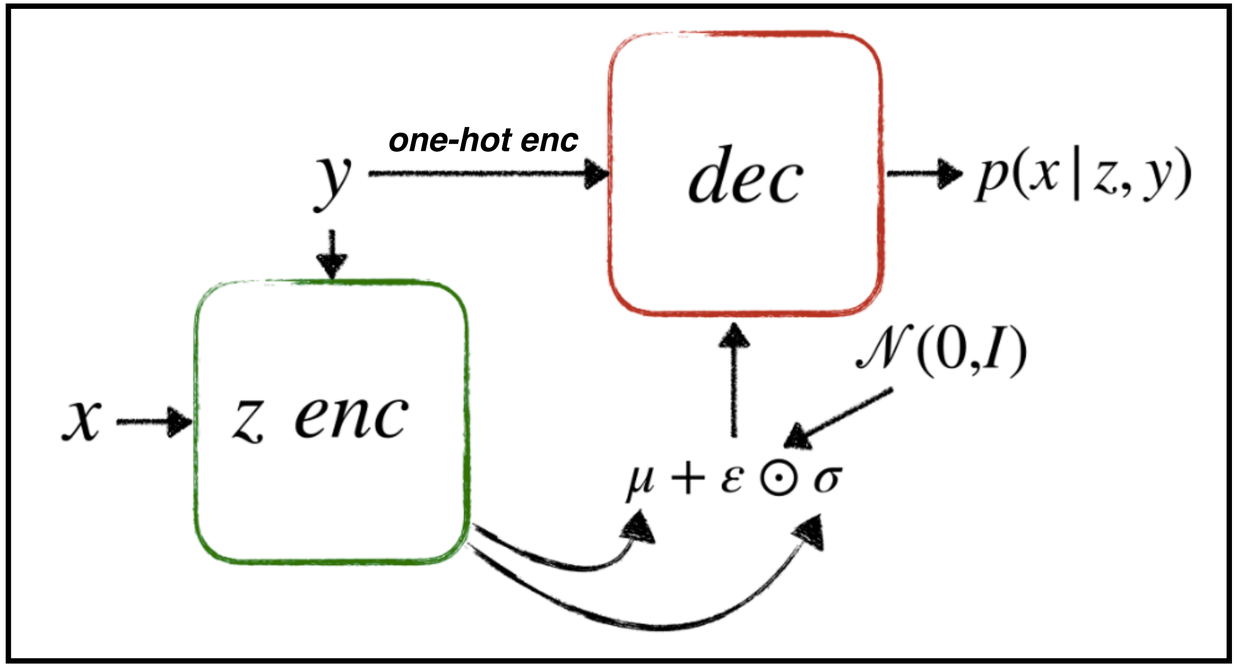
$$\frac{1}{|P|} \sum_{i \in P} y_i^T \log q(y \mid x).$$

SS-VAE: computational graph

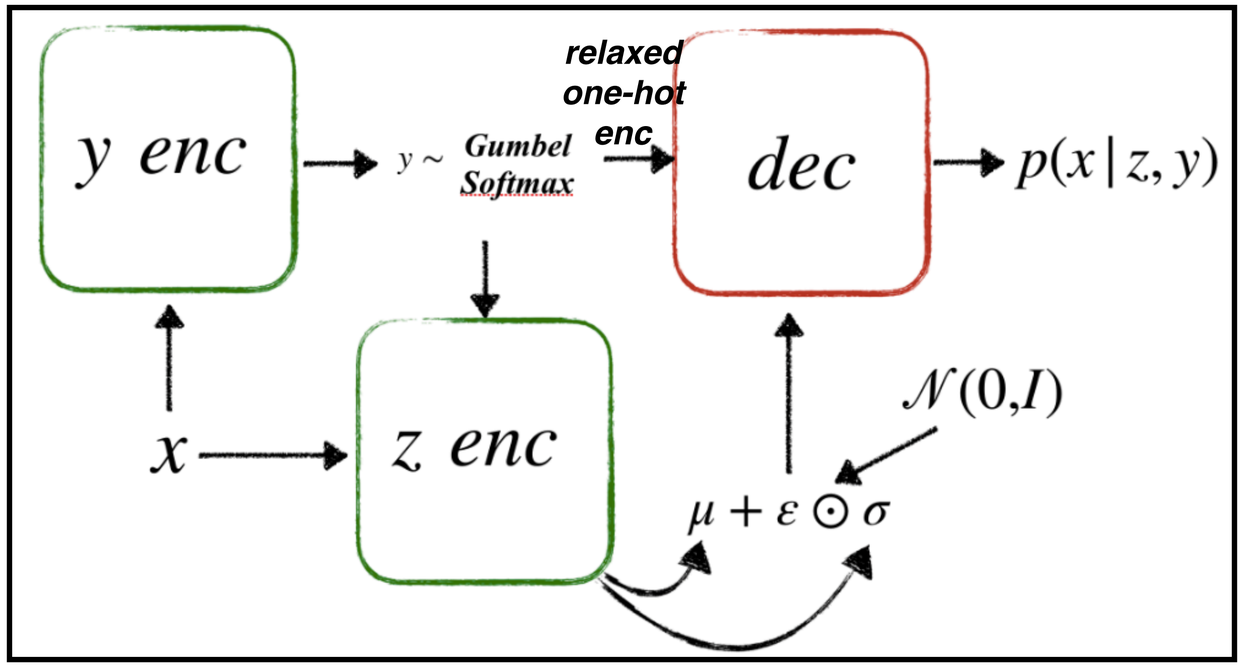
For vanilla VAE:



For observed labels (similar to VAE):



For unobserved labels:



SS-VAE: code: preprocessing data

1. Remove 95% of labels from the training set.
2. The observed labels have a standard one-hot encoding.
3. The unobserved labels are represented by all-zero ten dimensional vectors.

```
data = MNIST(root='.', download=True, train=True)
new_train_labels = torch.zeros(60000, 10)
observed = np.random.choice(60000, 3000)
new_train_labels[observed] = torch.eye(10)[data.targets][observed]
train_data = TensorDataset(data.data.view(-1, 28 * 28).float() / 255,
                           new_train_labels)

data = MNIST(root='.', download=True, train=False)
test_data = TensorDataset(data.data.view(-1, 28 * 28).float() / 255,
                          data.targets)
```

SS-VAE: code: defining encoders and decoder

```
n_classes, d, nh, D = 10, 32, 500, 28 * 28
default_T = torch.tensor(0.6, device=device)

yz_dec = nn.Sequential(
    nn.Linear(n_classes + d, nh),
    nn.ReLU(),
    nn.Linear(nh, D))

y_enc = nn.Sequential(
    nn.Linear(D, nh),
    nn.ReLU(),
    nn.Linear(nh, n_classes))

z_enc = nn.Sequential(
    nn.Linear(n_classes + D, nh),
    nn.ReLU(),
    nn.Linear(nh, 2 * d)
    )

yz_dec = yz_dec.to(device)
y_enc = y_enc.to(device)
z_enc = z_enc.to(device)
```

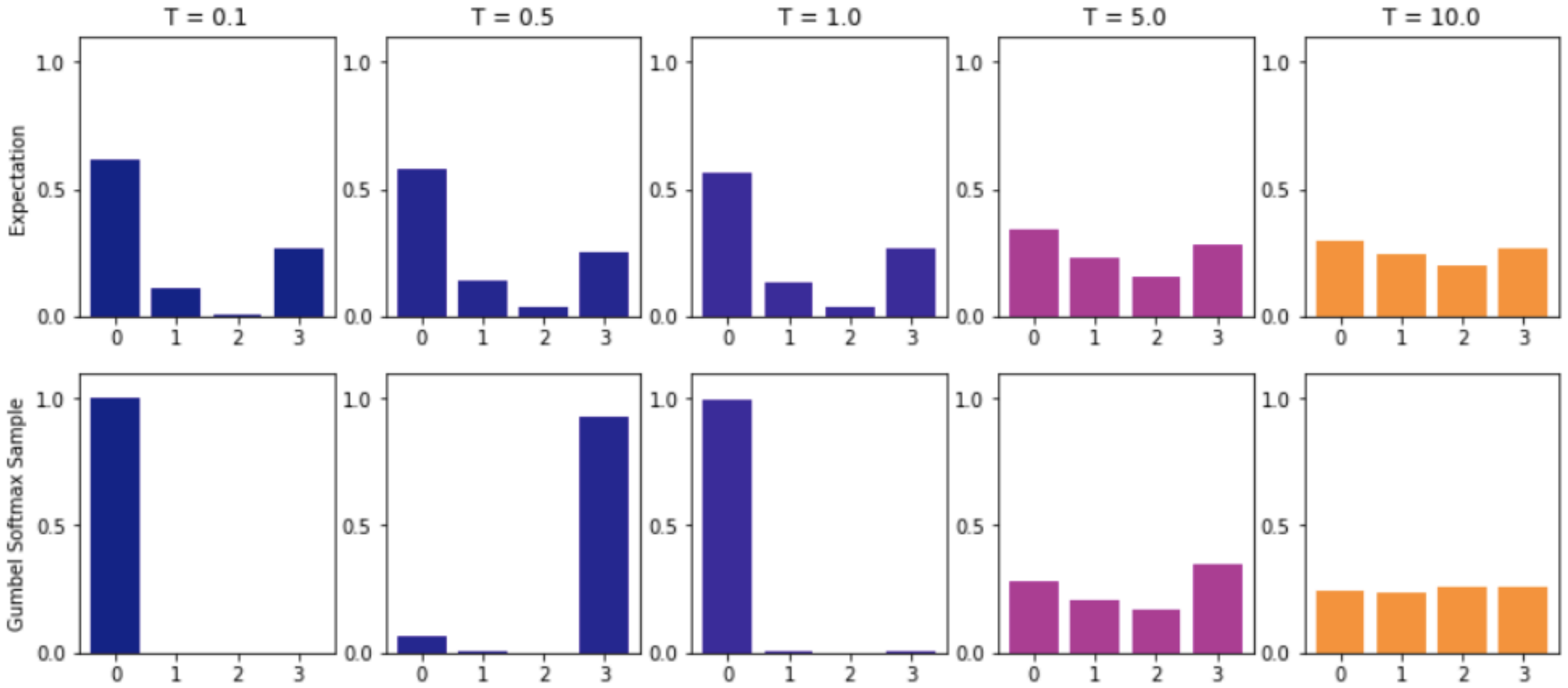
SS-VAE: code: computing loss

```
def loss(x, y, y_encoder, z_encoder, decoder, T=default_T, alpha=32.):
    #TODO
    """
    NOTE:
      hyperparameter alpha was tuned for the implementation that computed
      the mean of elbo terms and sum of cross-entropy terms over the observed
      datapoints in the batch

      In the modified training set the observed labels have a standard one-hot
      encoding and the unobserved labels are represented by all-zero ten
      dimensional vectors.
      To compute the mask for observed labels you can compute
      y_is_observed = y.sum(1, keepdim=True)

    The function has to
    1. sample y from q(y | x)
    2. sample z from q(z | x, y)
    3. compute the evidence lower bound for obervsed and unobserved variables
    4. compute the cross_entropy regularizer with weight alpha for object with
      observed labels
    5. return the sum of two losses
    """
```

Gumbel softmax trick: example

```
from torch.distributions.relaxed_categorical import RelaxedOneHotCategorical
n_classes = 4
logits = torch.randn(1, n_classes)
print('Probs: ', torch.nn.functional.softmax(logits, 1).squeeze().numpy())
temperatures = [0.1, 0.5, 1., 5., 10.]
M = 128

for n, t in enumerate(temperatures):
    dist = RelaxedOneHotCategorical(t, logits=logits)
    mean = torch.zeros_like(logits)
    for _ in range(M):
        mean += dist.sample() / M
    sample = dist.sample()
```

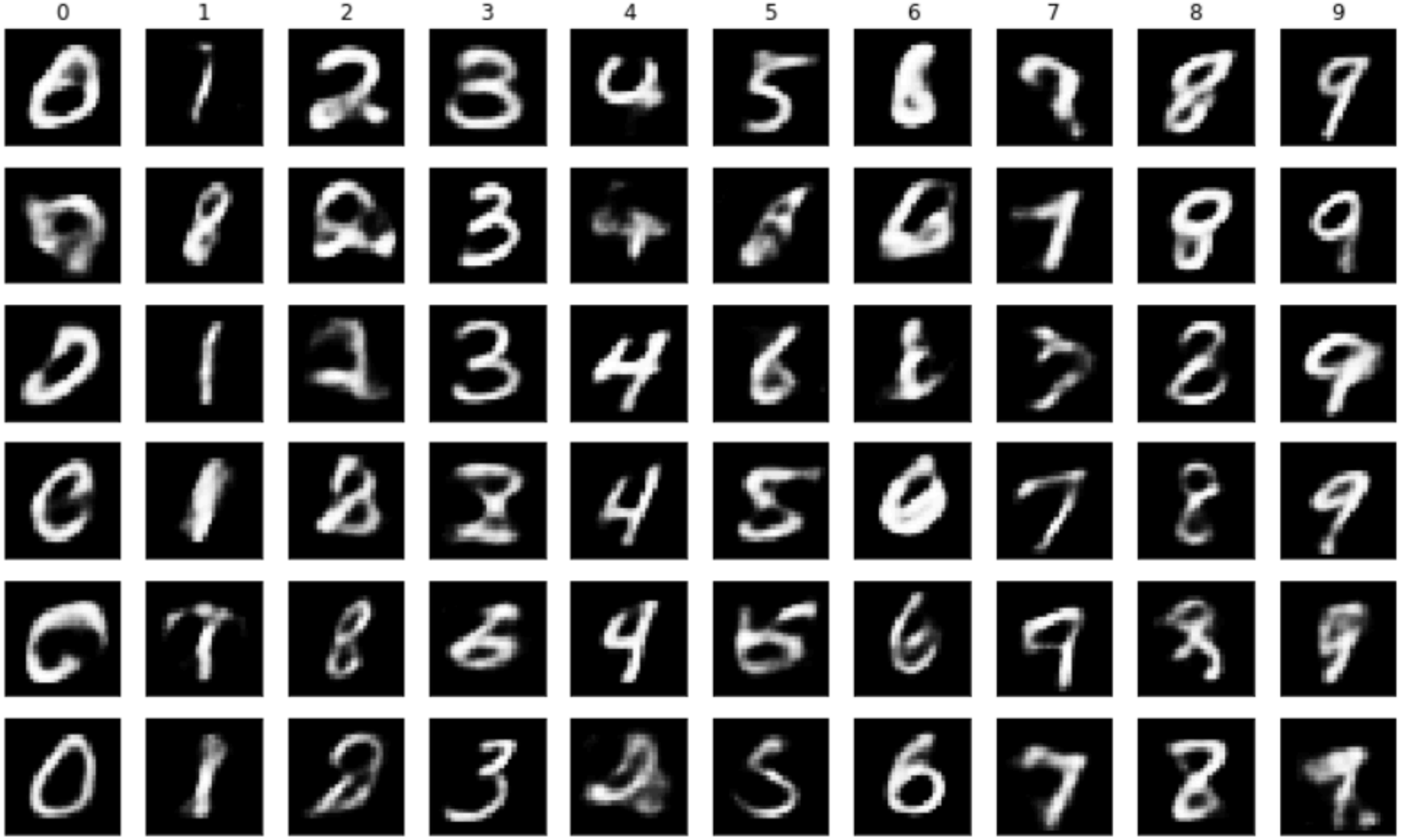
Gumbel softmax trick: example



Link to the task

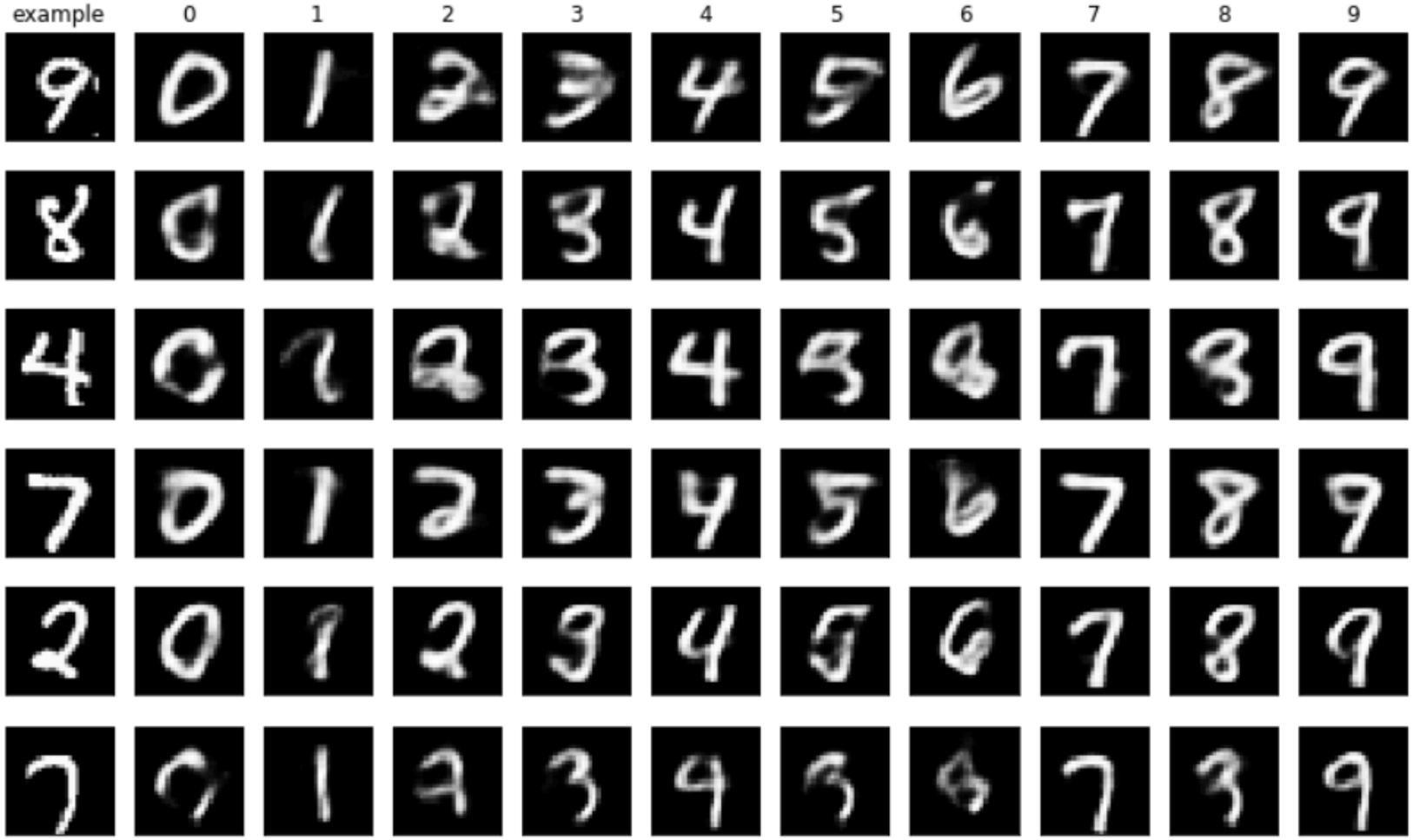
https://github.com/nadiinchi/ss_vae

Results: samples

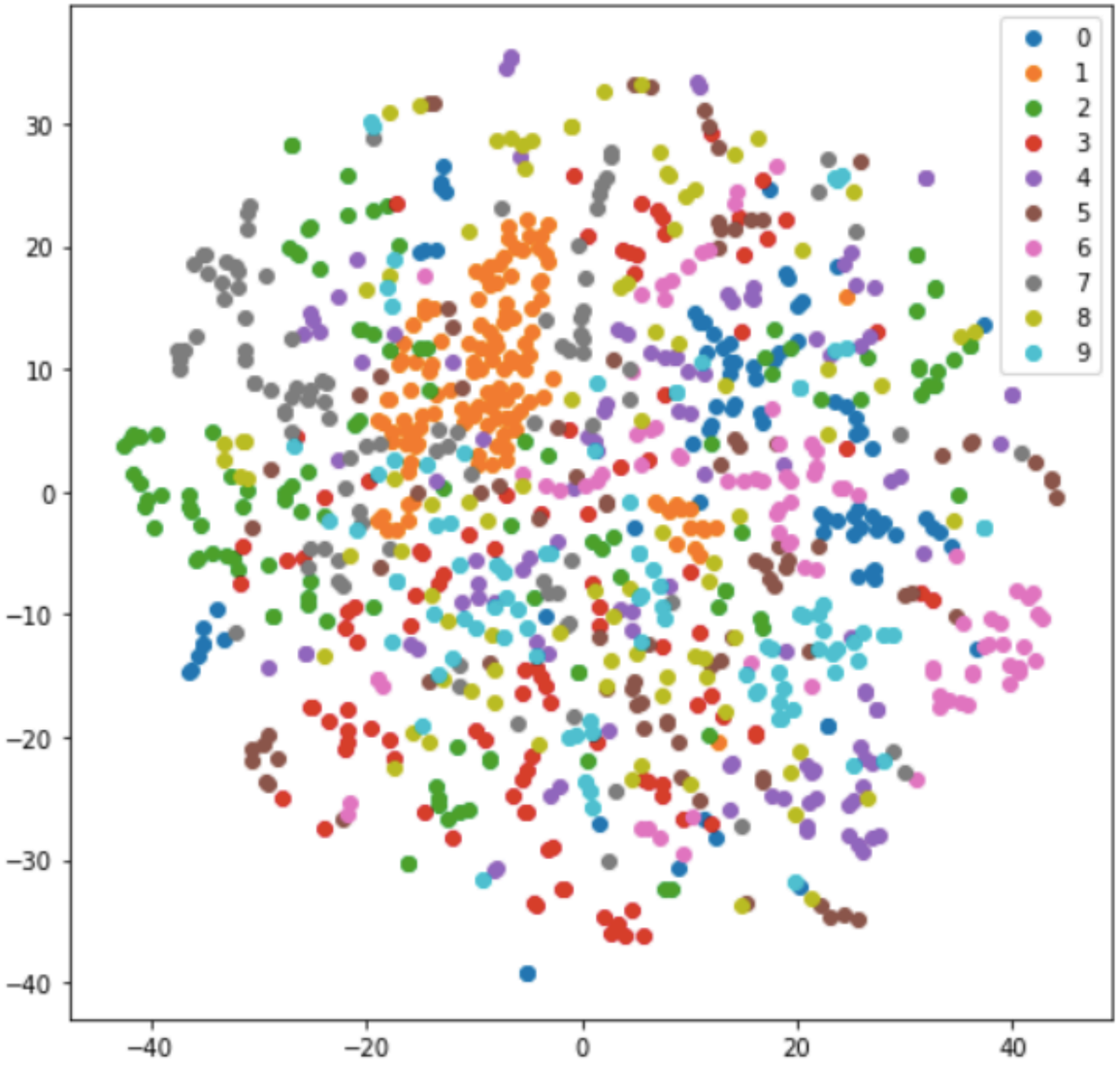


Results:”style transfer”

Infer latent representation z of a given digit x and then generate from p(x | z, y) for different y.



Results: tSNE of the latent space



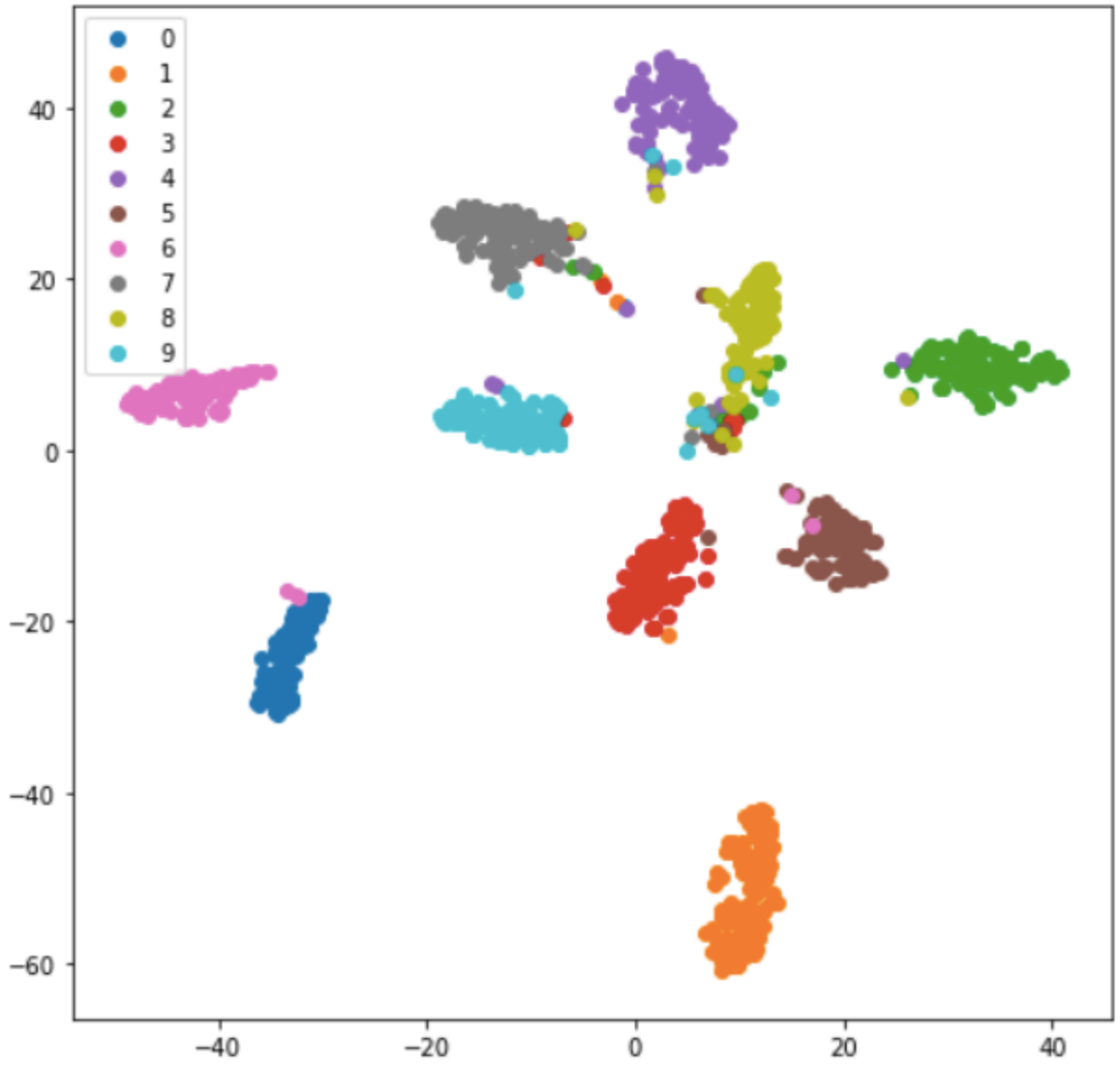
tSNE for q(z | x, y) mean values

↑

Gaussian distr.

Why mixed?

Results: tSNE of the class logits



tSNE for q(y | x) logits