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Problem 1

Formula for part 1 to 4

1. Log likelihood for Bernoulli distribution

For ONE sample, the log likelihood for this sample given the target is:

$$L(\mu) = \sum_{i=1}^n (\log \mu_i * target_i + \log 1 - \mu_i * (1 - target_i))$$

where $i = 1$ to n is the index for each pixel. And we will sum this formula by the dimension of batch, which is 1.

2. Log likelihood for Normal distribution

result = np.log(2*np.pi) + logvar + (z - mu).pow(2) / logvar.exp() result = (-1. / 2.) *
torch.sum(result, dim=1) # sum by batch Similarly, per sample, before we take on the log:

$$L(\mu) = \prod_i \left(\frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{(\mu - target)^2}{2\sigma^2}\right) \right)$$

Now if we take the log:

$$Log_L(\mu) = \sum_i -\frac{1}{2} \left(\log(2\pi\sigma) + \frac{(\mu - target)^2}{2\sigma^2} \right)$$

3. Log mean exp

Just follow the instruction. Build array A by taking the max on y, the rest is trivial

4. KL divergence

The formula for KL divergence, when p, q are both assumed Gaussian, has a neat form:

$$D_{KL}(p(x)||q(x)) = \sum_{x \in X} p(x) \log \frac{p(x)}{q(x)}$$

Now given $p(x) = \frac{1}{\sqrt{2\pi\sigma_p}} \exp(-(x - \mu_p)^2/2\sigma_p^2)$ and

$q(x) = \frac{1}{\sqrt{2\pi\sigma_q}} \exp(-(x - \mu_q)^2/2\sigma_q^2)$

$$p(x)/q(x) = \frac{\sqrt{\sigma_q}}{\sqrt{\sigma_p}} \exp[(x - \mu_p)^2/2\sigma_p^2 - (x - \mu_q)^2/2\sigma_q^2]$$

$$\log p(x)/q(x) = \frac{1}{2} * (\log var_q - \log var_p) + (\mu_p - \mu_q)^2 - (\log var_p^2 - \log var_q^2)$$

And we simply need to sum this up following axis 1 (batch)

Training result

6.

I have trained the model described in this notebook, with the log loss I implemented in the `vae.ipynb` whose PDF is attached at the end of Appendix. The result is shown above. And I have achieved an average per-instance ELBO of **101.28** at the end of 20-th epoch.

7.

The log-likelihood in test samples are **95.54**

Problem 2

1.

According to Equation 7 in the paper (Nowozin et al. link: <https://arxiv.org/pdf/1606.00709.pdf>), the objective is given as:

$$F(\theta, \omega) = E_{x \sim P}[g_f(V_\omega(x))] + E_{x \sim Q_\theta}[-f^*(V_\omega(x))]$$

Where g_f is the output activation function and f^* is the Conjugate function for Squared Hellinger:

$$g_f(v) = 1 - \exp(-v)$$
$$f^*(t) = \frac{t}{1 - t}$$

3.

The objective function of the Wasserstein distance is given as the Equation (5) in the paper by Petzka et al. (<https://arxiv.org/pdf/1709.08894.pdf> (<https://arxiv.org/pdf/1709.08894.pdf>)):

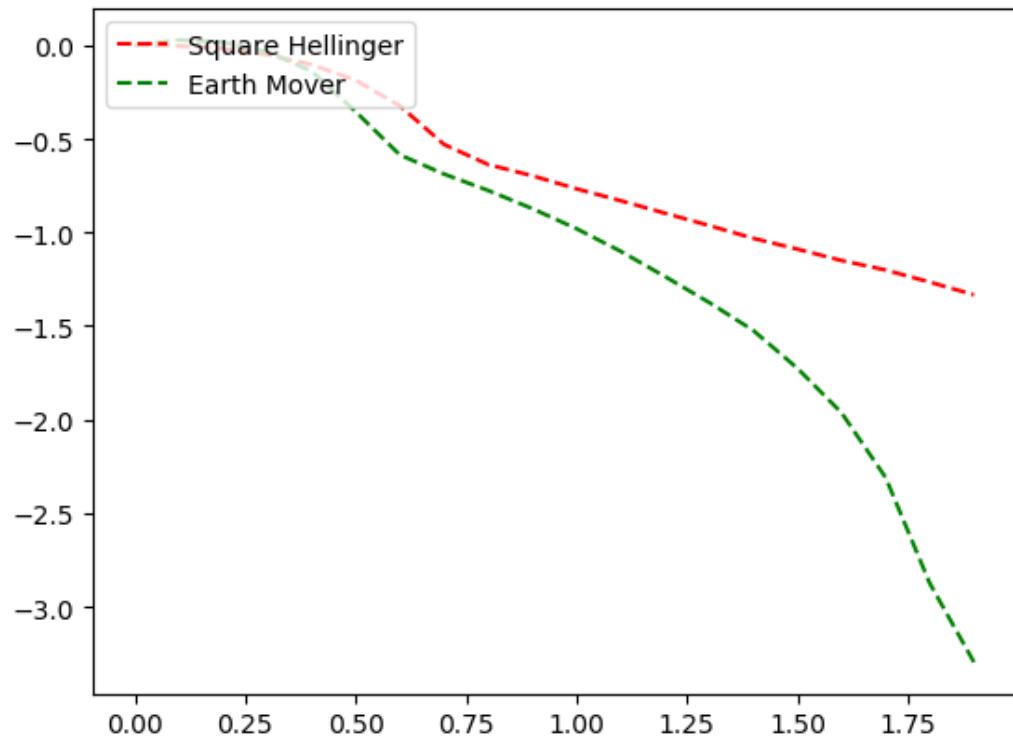
$$\min_v \max_{f \in Lip_1} E_{x \sim \mu}[f(x)] - E_{y \sim \nu}[f(y)]$$

Where the Lipschitz Penalty is defined as (equation 8 in the paper):

$$E_{y \sim \nu}[f(y)] - E_{x \sim \mu}[f(x)] + \lambda E_{\hat{x} \sim \tau}[(\max\{0, \|\nabla f(\hat{x})\| - 1\})^2]$$

5.

In this part we trained a toy model to uncover the variable theta. For each of distance of our choosing, we trained the same model for 30 epochs.



The distance vs. Theta is shown above, for Squared Hellinger and Earth Mover.

Problem 3

Samples

I have completed the training and sampling process given the code templates. Below are generated images from a generator that is trained for 150 epochs:



Blurriness

From the sampled pictures, we can see that the clarity of them are not comparable to the authentic ones. The major flaws are:

- The picture doesn't have the fine textures one would expect from wall or door materials.
- Half of the number signs were not readable.

Further training could probably help, 150 epochs may not be enough for this model.

Diversity

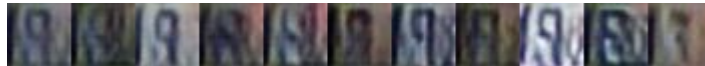
On the variety side, the generated samples did reflect a lot of differences in color and style.

Disentangled representation

I sampled a baseline seed z , and its image decoded were shown below:

Then for the 100 latent variable dimensions, I sampled every 10th of them and added 5.0 to the dimension, the generated images are shown below:

- the first picture is generated with baseline z
- the next ones are generated with some z 's components added by 5.0



From the pictures we can conclude that the model learned disentangled representations. Modifications to some components definitely changed the shape of writing.

Interpolating in two spaces

(a)

The images for $\alpha = 0, 0.1, 0.2, 0.3, 0.4, \dots, 1$ are shown below. We can see the writing of 7 gradually changed to 1.



(b)

The images by interpolating directly in the data space are shown below. The clarity is not as good as the first one because these images are simply overlaid.



Appendix

Image generation code (auxiliary)

```
In [ ]: 1 # Auxiliary code for image generations
2
3 import torch
4 import numpy as np
5 from torchvision import transforms, datasets
6 from torch.utils.data.sampler import SubsetRandomSampler
7 from torch import nn
8 from torch import optim
9 import math
10 import matplotlib.pyplot as plt
11
12 device = 'cuda' if torch.cuda.is_available() else 'cpu'
13
14 generator = torch.load("generator3.pt")
15 critic = torch.load("critic3.pt")
16 generator.eval()
17 critic.eval()
```

```
In [ ]: 1 import scipy
2 import math
3 import matplotlib.pyplot as plt
4
5 def generate_samples(model, size=36, plot=True, path='figures/'):
6     with torch.no_grad():
7         images = model.generate(torch.randn(size, 100).to(device)).cpu().numpy()
8         images = np.moveaxis(images, 1, 3)
9         rows = []
10        how_many_per_row = int(np.sqrt(size))
11        for i in range(how_many_per_row):
12            rows.append(
13                np.hstack([images[j] for j in range(i*how_many_per_row, (i+1)*how_many_per_row)])
14            )
15        big_picture = np.vstack(rows)
16
17        scipy.misc.imsave(f"{path}/big_picture2.jpg", big_picture)
18 # COMPLETE QUALITATIVE EVALUATION
19 generate_samples(generator, size=100)
```

```
In [ ]: 1 baseline_z = torch.randn(1, 100).cpu().detach().numpy()
2 # get ten copies for perturb
3 baseline_z = np.repeat(baseline_z, 11, axis = 0)
4 for row, dim in enumerate(range(0,100,10)):
5     print(row, dim)
6     baseline_z[row+1][dim] += 5
7
8
9 def generate_z_axis(model, path="figures/"):
10     with torch.no_grad():
11         # generate_baseline_model
12         images = model.generate(torch.from_numpy(baseline_z).to(device)).cpu().numpy()
13         images = np.moveaxis(images, 1, 3)
14         scipy.misc.imsave(f"{path}/z_disentangled.jpg", np.hstack([images[i] for i in range(0,10)]))
15
16 generate_z_axis(generator)
```

```
In [ ]: 1 baseline_z0 = torch.randn(2, 100).cpu().detach().numpy()
2
3 def generate_image_space_interp(model, path="figures/"):
4     with torch.no_grad():
5         # generate_baseline_model
6         images = model.generate(torch.from_numpy(baseline_z0).to(device))
7         images = np.moveaxis(images, 1, 3)
8         interp = [
9             images[0] * (10-i)/10 + images[1] * (i/10)
10            for i in range(10)
11        ]
12        scipy.misc.imsave(f"{path}/image_space.jpg", np.hstack(interp))
13
14 generate_image_space_interp(generator)
```

vae.ipynb, completed

Solution template for the question 1.6-1.7. This template consists of following steps. Except the step 2, you don't need to modify it to answer the questions.

1. Initialize libraries
2. **Insert the answers for the questions 1.1~1.5 below (this is the part you need to fill)**
3. Define data loaders
4. Define VAE network architecture
5. Initialize the model and optimizer
6. Train the model
7. Save the model
8. Load the model
9. Evaluate the model with importance sampling

Initialize libraries

```
In [1]: 1 import math
        2 from torchvision.datasets import utils
        3 import torch.utils.data as data_utils
        4 import torch
        5 import os
        6 import numpy as np
        7 from torch import nn
        8 from torch.nn.modules import upsampling
        9 from torch.functional import F
       10 from torch.optim import Adam
```

Insert **the answers for the questions 1.1~1.5 below**

In [2]:

```
1 def log_likelihood_bernoulli(mu, target):
2     """
3     COMPLETE ME. DONT MODIFY THE PARAMETERS OF THE FUNCTION. Otherw
4
5     *** note. ***
6
7     :param mu: (FloatTensor) - shape: (batch_size x input_size) - T
8     :param target: (FloatTensor) - shape: (batch_size x input_size)
9     :return: (FloatTensor) - shape: (batch_size,) - log-likelihood
10    """
11    # init
12    batch_size = mu.size(0)
13    mu = mu.view(batch_size, -1)
14    target = target.view(batch_size, -1)
15    result = target * torch.log(mu) + (1 - target) * torch.log(1 -
16    result = torch.sum(result, dim=1)
17    return result
18
19 def log_likelihood_normal(mu, logvar, z):
20     """
21     COMPLETE ME. DONT MODIFY THE PARAMETERS OF THE FUNCTION. Otherw
22
23     *** note. ***
24
25     :param mu: (FloatTensor) - shape: (batch_size x input_size) - T
26     :param logvar: (FloatTensor) - shape: (batch_size x input_size)
27     :param z: (FloatTensor) - shape: (batch_size x input_size) - Ta
28     :return: (FloatTensor) - shape: (batch_size,) - log probability
29    """
30    # init
31    batch_size = mu.size(0)
32    mu = mu.view(batch_size, -1)
33    logvar = logvar.view(batch_size, -1)
34    z = z.view(batch_size, -1)
35    part_a = np.log(2 * np.pi) + logvar
36    part_b = (z - mu).pow(2) / logvar.exp()
37    result = (-1.0 / 2.0) * torch.sum(part_a + part_b, dim=1) # su
38    return result
39
40 def log_mean_exp(y):
41     """
42     COMPLETE ME. DONT MODIFY THE PARAMETERS OF THE FUNCTION. Otherw
43
44     *** note. ***
45
46     :param y: (FloatTensor) - shape: (batch_size x sample_size) - V
47     :return: (FloatTensor) - shape: (batch_size,) - Output for log_
48    """
49    # init
50    batch_size = y.size(0)
51    sample_size = y.size(1)
52
53    # log_mean_exp
54
55    a_array = y.max(dim=1, keepdim=True)[0]
56    exp_y = (y - a_array).exp()
```



```

57     sum_exp = torch.sum(exp_y, dim=1) # sum by batch size
58     result = (1.0 / sample_size * sum_exp).log() + a_array.view(-1)
59     return result
60
61
62 def kl_gaussian_gaussian_analytic(mu_q, logvar_q, mu_p, logvar_p):
63     """
64     COMPLETE ME. DONT MODIFY THE PARAMETERS OF THE FUNCTION. Otherwise
65
66     *** note. ***
67
68     :param mu_q: (FloatTensor) - shape: (batch_size x input_size) -
69     :param logvar_q: (FloatTensor) - shape: (batch_size x input_size) -
70     :param mu_p: (FloatTensor) - shape: (batch_size x input_size) -
71     :param logvar_p: (FloatTensor) - shape: (batch_size x input_size) -
72     :return: (FloatTensor) - shape: (batch_size,) - kl-divergence of
73     """
74     # init
75     batch_size = mu_q.size(0)
76     mu_q = mu_q.view(batch_size, -1)
77     logvar_q = logvar_q.view(batch_size, -1)
78     mu_p = mu_p.view(batch_size, -1)
79     logvar_p = logvar_p.view(batch_size, -1)
80
81     pq = (
82         logvar_p
83         - logvar_q
84         - 1.0
85         + (logvar_q.exp() / logvar_p.exp())
86         + ((mu_q - mu_p).pow(2) / logvar_p.exp())
87     )
88     result = (1.0 / 2.0) * torch.sum(pq, dim=1)
89     return result
90
91 def kl_gaussian_gaussian_mc(mu_q, logvar_q, mu_p, logvar_p, num_samples):
92     """
93     COMPLETE ME. DONT MODIFY THE PARAMETERS OF THE FUNCTION. Otherwise
94
95     *** note. ***
96
97     :param mu_q: (FloatTensor) - shape: (batch_size x input_size) -
98     :param logvar_q: (FloatTensor) - shape: (batch_size x input_size) -
99     :param mu_p: (FloatTensor) - shape: (batch_size x input_size) -
100    :param logvar_p: (FloatTensor) - shape: (batch_size x input_size) -
101    :param num_samples: (int) - shape: () - The number of sample for
102    :return: (FloatTensor) - shape: (batch_size,) - kl-divergence of
103    """
104    # init
105    batch_size = mu_q.size(0)
106    input_size = np.prod(mu_q.size()[1:])
107    mu_q = (
108        mu_q.view(batch_size, -1)
109        .unsqueeze(1)
110        .expand(batch_size, num_samples, input_size)
111    )
112    logvar_q = (
113        logvar_q.view(batch_size, -1)

```

```

114         .unsqueeze(1)
115         .expand(batch_size, num_samples, input_size)
116     )
117     mu_p = (
118         mu_p.view(batch_size, -1)
119         .unsqueeze(1)
120         .expand(batch_size, num_samples, input_size)
121     )
122     logvar_p = (
123         logvar_p.view(batch_size, -1)
124         .unsqueeze(1)
125         .expand(batch_size, num_samples, input_size)
126     )
127
128     # ==
129     # Monte carlo kld
130
131     # define the normal distribution to sample from
132     stdev_q = (0.5 * logvar_q).exp()
133     normal = torch.distributions.Normal(mu_q.float(), stdev_q.float())
134     sampled_x = normal.sample()
135     f_q = logvar_q + (sampled_x - mu_q).pow(2) / logvar_q.exp()
136     f_p = logvar_p + (sampled_x - mu_p).pow(2) / logvar_p.exp()
137     q_p = f_q - f_p
138     sampled_x_KL = torch.sum(q_p, dim=2)
139     kld = -0.5 / num_samples * torch.sum(sampled_x_KL, dim=1)
140     return kld

```

Define data loaders

```

In [3]: 1 def get_data_loader(dataset_location, batch_size):
2         URL = "http://www.cs.toronto.edu/~larocche/public/datasets/binarized_mnist_%s.amat" % splitname
3         # start processing
4         def lines_to_np_array(lines):
5             return np.array([[int(i) for i in line.split()] for line in lines])
6         splitdata = []
7         for splitname in ["train", "valid", "test"]:
8             filename = "binarized_mnist_%s.amat" % splitname
9             filepath = os.path.join(dataset_location, filename)
10            utils.download_url(URL + filename, dataset_location)
11            with open(filepath) as f:
12                lines = f.readlines()
13            x = lines_to_np_array(lines).astype('float32')
14            x = x.reshape(x.shape[0], 1, 28, 28)
15            # pytorch data loader
16            dataset = data_utils.TensorDataset(torch.from_numpy(x))
17            dataset_loader = data_utils.DataLoader(x, batch_size=batch_size)
18            splitdata.append(dataset_loader)
19        return splitdata

```

```
In [4]: 1 train, valid, test = get_data_loader("binarized_mnist", 64)
```

Downloading http://www.cs.toronto.edu/~larocheh/public/datasets/binarized_mnist/binarized_mnist_train.amat (http://www.cs.toronto.edu/~larocheh/public/datasets/binarized_mnist/binarized_mnist_train.amat) to binarized_mnist/binarized_mnist_train.amat

78405632/? [00:20<00:00, 8440060.34it/s]

Downloading http://www.cs.toronto.edu/~larocheh/public/datasets/binarized_mnist/binarized_mnist_valid.amat (http://www.cs.toronto.edu/~larocheh/public/datasets/binarized_mnist/binarized_mnist_valid.amat) to binarized_mnist/binarized_mnist_valid.amat

15687680/? [00:20<00:00, 8121116.75it/s]

Downloading http://www.cs.toronto.edu/~larocheh/public/datasets/binarized_mnist/binarized_mnist_test.amat (http://www.cs.toronto.edu/~larocheh/public/datasets/binarized_mnist/binarized_mnist_test.amat) to binarized_mnist/binarized_mnist_test.amat

15687680/? [00:03<00:00, 5080611.19it/s]

Define VAE network architecture

```

In [5]: 1 class Encoder(nn.Module):
2         def __init__(self, latent_size):
3             super(Encoder, self).__init__()
4             self.mlp = nn.Sequential(
5                 nn.Linear(784, 300),
6                 nn.ELU(),
7                 nn.Linear(300, 300),
8                 nn.ELU(),
9                 nn.Linear(300, 2 * latent_size),
10            )
11
12        def forward(self, x):
13            batch_size = x.size(0)
14            z_mean, z_logvar = self.mlp(x.view(batch_size, 784)).chunk(2)
15            return z_mean, z_logvar
16
17    class Decoder(nn.Module):
18        def __init__(self, latent_size):
19            super(Decoder, self).__init__()
20            self.mlp = nn.Sequential(
21                nn.Linear(latent_size, 300),
22                nn.ELU(),
23                nn.Linear(300, 300),
24                nn.ELU(),
25                nn.Linear(300, 784),
26            )
27
28        def forward(self, z):
29            return self.mlp(z) - 5.
30
31    class VAE(nn.Module):
32        def __init__(self, latent_size):
33            super(VAE, self).__init__()
34            self.encode = Encoder(latent_size)
35            self.decode = Decoder(latent_size)
36
37        def forward(self, x):
38            z_mean, z_logvar = self.encode(x)
39            z_sample = z_mean + torch.exp(z_logvar / 2.) * torch.randn(
40                z_mean.size())
41            x_mean = self.decode(z_sample)
42            return z_mean, z_logvar, x_mean
43
44        def loss(self, x, z_mean, z_logvar, x_mean):
45            ZERO = torch.zeros(z_mean.size())
46            #kl = kl_gaussian_gaussian_mc(z_mean, z_logvar, ZERO, ZERO,
47            kl = kl_gaussian_gaussian_analytic(z_mean, z_logvar, ZERO,
48            recon_loss = -log_likelihood_bernoulli(
49                torch.sigmoid(x_mean.view(x.size(0), -1)),
50                x.view(x.size(0), -1),
51            ).mean()
52            return recon_loss + kl

```

Initialize a model and optimizer

```
In [6]: 1 vae = VAE(100)
        2 params = vae.parameters()
        3 optimizer = Adam(params, lr=3e-4)
        4 print(vae)
```

```
VAE(
  (encode): Encoder(
    (mlp): Sequential(
      (0): Linear(in_features=784, out_features=300, bias=True)
      (1): ELU(alpha=1.0)
      (2): Linear(in_features=300, out_features=300, bias=True)
      (3): ELU(alpha=1.0)
      (4): Linear(in_features=300, out_features=200, bias=True)
    )
  )
  (decode): Decoder(
    (mlp): Sequential(
      (0): Linear(in_features=100, out_features=300, bias=True)
      (1): ELU(alpha=1.0)
      (2): Linear(in_features=300, out_features=300, bias=True)
      (3): ELU(alpha=1.0)
      (4): Linear(in_features=300, out_features=784, bias=True)
    )
  )
)
```

Train the model

```
In [7]: 1 for i in range(20):
2         # train
3         for x in train:
4             optimizer.zero_grad()
5             z_mean, z_logvar, x_mean = vae(x)
6             loss = vae.loss(x, z_mean, z_logvar, x_mean)
7             loss.backward()
8             optimizer.step()
9
10        # evaluate ELBO on the valid dataset
11        with torch.no_grad():
12            total_loss = 0.
13            total_count = 0
14            for x in valid:
15                total_loss += vae.loss(x, *vae(x)) * x.size(0)
16                total_count += x.size(0)
17            print('-elbo: ', (total_loss / total_count).item())
```

```
-elbo: 167.884521484375
-elbo: 142.44168090820312
-elbo: 129.18482971191406
-elbo: 121.11119079589844
-elbo: 115.97421264648438
-elbo: 113.12680053710938
-elbo: 110.89364624023438
-elbo: 109.18376159667969
-elbo: 107.71327209472656
-elbo: 106.6328353881836
-elbo: 105.85040283203125
-elbo: 105.10814666748047
-elbo: 104.2016830444336
-elbo: 103.8462905883789
-elbo: 102.88982391357422
-elbo: 102.59537506103516
-elbo: 102.35488891601562
-elbo: 101.95604705810547
-elbo: 101.50086212158203
-elbo: 101.28077697753906
```

Save the model

```
In [8]: 1 torch.save(vae, 'model.pt')
```

```
/home/andybai/anaconda3/lib/python3.7/site-packages/torch/serializatio
n.py:360: UserWarning: Couldn't retrieve source code for container of
type VAE. It won't be checked for correctness upon loading.
  "type " + obj.__name__ + ". It won't be checked "
/home/andybai/anaconda3/lib/python3.7/site-packages/torch/serializatio
n.py:360: UserWarning: Couldn't retrieve source code for container of
type Encoder. It won't be checked for correctness upon loading.
  "type " + obj.__name__ + ". It won't be checked "
/home/andybai/anaconda3/lib/python3.7/site-packages/torch/serializatio
n.py:360: UserWarning: Couldn't retrieve source code for container of
type Decoder. It won't be checked for correctness upon loading.
  "type " + obj.__name__ + ". It won't be checked "
```

Load the model

```
In [9]: 1 vae = torch.load('model.pt')
```

Evaluate the $\log p_{\theta}(x)$ of the model on test by using importance sampling

```
In [11]: 1 total_loss = 0.  
2 total_count = 0  
3 with torch.no_grad():  
4     #x = next(iter(test))  
5     for x in test:  
6         # init  
7         K = 200  
8         M = x.size(0)  
9  
10        # Sample from the posterior  
11        z_mean, z_logvar = vae.encode(x)  
12        eps = torch.randn(z_mean.size(0), K, z_mean.size(1))  
13        z_samples = z_mean[:, None, :] + torch.exp(z_logvar / 2.):  
14  
15        # Decode samples  
16        z_samples_flat = z_samples.view(-1, z_samples.size(-1)) # F  
17        x_mean_flat = vae.decode(z_samples_flat) # Push it through  
18  
19        # Reshape images and posterior to evaluate probabilities  
20        x_flat = x[:, None].repeat(1, K, 1, 1, 1).reshape(M*K, -1)  
21        z_mean_flat = z_mean[:, None, :].expand_as(z_samples).resha  
22        z_logvar_flat = z_logvar[:, None, :].expand_as(z_samples).  
23        ZEROS = torch.zeros(z_mean_flat.size())  
24  
25        # Calculate all the probabilities!  
26        log_p_x_z = log_likelihood_bernoulli(torch.sigmoid(x_mean_f  
27        log_q_z_x = log_likelihood_normal(z_mean_flat, z_logvar_fla  
28        log_p_z = log_likelihood_normal(ZEROS, ZEROS, z_samples_fla  
29  
30        # Recombine them.  
31        w = log_p_x_z + log_p_z - log_q_z_x  
32        log_p = log_mean_exp(w)  
33  
34        # Accumulate  
35        total_loss += log_p.sum()  
36        total_count += M  
37        print('log p(x):', (total_loss / total_count).item())
```

log p(x): -95.54447174072266