VAE MNIST StaticPlot

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- 1 MLP Variational Autoencoder for MNIST dataset
- 2 +
- 3 Static plots for training and latent interpolation

implement probability and sampling with torch.distribution package, modified from this link

```
[1]: %matplotlib inline
     import os, sys
     import numpy as np
     import pickle
     import matplotlib.pyplot as plt
     import warnings
     warnings.filterwarnings("ignore")
     import torch
     import torch.nn as nn
     import torch.nn.functional as F
     import torch.optim as optim
     import torchvision
     import torch.distributions as torchD
     import torch, seaborn as sns
     import pandas as pd
     from mpl_toolkits.mplot3d import Axes3D
     from matplotlib.colors import ListedColormap
     from utils import *
```

```
[2]: # # set seed for reproducibility
# seed = 24
# torch.manual_seed(seed)
# np.random.seed(seed)
```

3.1 Load Dataset

```
[3]: # !wget www.di.ens.fr/~lelarge/MNIST.tar.gz
# !tar -zxvf MNIST.tar.gz
```

3.2 Variational Autoencoder

A MLP variational autoencoder is used. The mean and s.d. of the approximate posterior are outputs of the encoding MLP. See more details at VAE paper

```
[7]: class MLP_VAE(nn.Module):
         TODO: check whether to use sum or mean for the probability part
         def __init__(self, **kwargs):
             # kwarqs["input shape"] = [1,28,28]
             # kwargs["latent_dim"] = 4
             super(MLP_VAE, self).__init__()
             self.encoder = MLP_V_Encoder(**kwargs)
             self.decoder = MLP_V_Decoder(**kwargs)
             # distribution layers
             self.enc_dim = kwargs["enc_dim"]
             self.latent_dim = kwargs["latent_dim"]
             self.enc_to_mean = nn.Linear(self.enc_dim, self.latent_dim)
             self.enc_to_logvar = nn.Linear(self.enc_dim, self.latent_dim)
         def encode(self, x):
             enc_out = self.encoder(x)
             mean = self.enc_to_mean(enc_out)
             logvar = self.enc_to_logvar(enc_out)
             return mean, logvar
         def decode(self, latent):
             return self.decoder(latent)
         def pxz likelihood(self, x, x_bar, scale=1., dist_type="Gaussian"):
             11 11 11
             compute the likelihood p(x/z) based on predefined distribution, given a_{\sqcup}
      \hookrightarrow latent vector z
             default scale = 1, can be broadcasted to the shape of x_bar
             if dist_type == "Gaussian":
                 dist = torch.distributions.Normal(loc=x_bar, scale=scale)
             else:
```

```
raise NotImplementedError("unknown distribution for p(x|z) {}".
→format(dist_type))
      log_pxz = dist.log_prob(x)
      return log_pxz.sum() # log_pxz.sum((1,2,3))
  def kl_divergence(self, mean, logvar):
      Monte Carlo way to solve KL divergence
      pz = torchD.Normal(torch.zeros_like(mean), scale=1)
      std = torch.exp(0.5*logvar)
      qzx = torchD.Normal(loc=mean, scale=std)
      z = qzx.rsample() # reparameterized sampling, shape [32,2]
       # clamp the log prob to avoid -inf
      qzx_lp = qzx.log_prob(z).clamp(min=-1e10, max=0.)
      pz_lp = pz.log_prob(z).clamp(min=-1e10, max=0.)
      kl = qzx_lp - pz_lp
      if torch.isnan(qzx_lp).any():
           print("nan in qzx_lp")
           print("qzx_lp")
           print(qzx_lp)
          print("z")
           print(z)
          print("mean")
           print(mean)
           print("logvar")
           print(logvar)
           plot_p_q(mean, logvar)
           raise ValueError
       if torch.isnan(pz_lp).any():
           print("nan in pz_lp")
           print("pz_lp")
           print(pz_lp)
           print("z")
           print(z)
           print("mean")
           print(mean)
           print("logvar")
           print(logvar)
           plot_p_q(mean, logvar)
           raise ValueError
      if torch.isnan(kl.mean()).any():
           print(qzx_lp)
```

```
print(pz_lp)
           print(z)
       return kl.sum()
   def reparameterize(self, mean, logvar):
       # assume Gaussian for p(epsilon)
       sd = torch.exp(0.5*logvar)
       # use randn_like to sample N(0,1) of the same size as std/mean
       # default only sample once, otherwise should try sample multiple times
\rightarrow take mean
       eps = torch.randn_like(sd)
       return mean + sd * eps
   def sample latent embedding(self, mean, logvar, method="reparameterize"):
       Write a sampling function to make function name consistent
       if method=="reparameterize":
           return self.reparameterize(mean, logvar)
       else:
           raise NotImplementedError("Unrecognized method for sampling latent ⊔
→embedding {}".format(method))
   def forward(self, x, if_plot_pq=False):
       latent_mean, latent_logvar = self.encode(x)
       latent = self.reparameterize(latent_mean, latent_logvar)
       x_bar = self.decoder(latent)
       if if_plot_pq:
           plot_p_q(latent_mean, latent_logvar)
       return latent, x_bar, latent_mean, latent_logvar
```

3.3 Training process

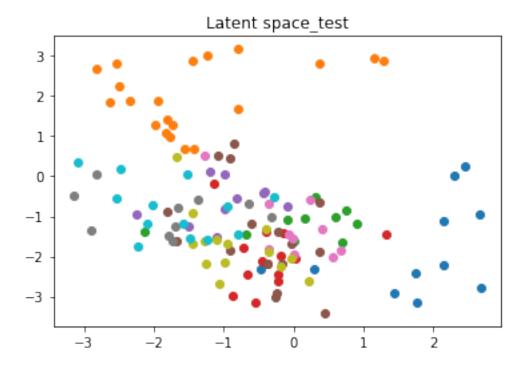
```
if use_scheduler:
       step_size = 5
       gamma = 0.1
       scheduler = optim.lr_scheduler.StepLR(optimizer, step_size=step_size,_
→gamma=gamma)
   epoch_train_loss = []
   epoch_train_kl_loss = []
   epoch_train_recon_loss = []
   epoch_sample_img = []
   epoch_sample_reconstruction = []
   epoch_sample_latent = []
   epoch_train_kl_divergence = []
   epoch_train_pxz_likelihood = []
   epoch_train_elbo = []
   model.train()
   for epoch in range(num_epochs):
       model.train()
       train_loss = 0
       train_kl_loss = 0
       train_recon_loss = 0
       train_kl_divergence = 0
       train_pxz_likelihood = 0
       train_elbo = 0
       for img, label in train_loader:
           optimizer.zero_grad()
           img, label = img.to(device), label.to(device)
           latent, reconstruction, latent_mean, latent_logvar = model(img)
           kl_loss = -0.5 * torch.sum(1 + latent_logvar - latent_mean.pow(2) -
→latent_logvar.exp())
           kl_divergence = model.kl_divergence(latent_mean, latent_logvar)
           recon_loss = recon_loss_fn(reconstruction, img)
           pxz_likelihood = model.pxz_likelihood(img, reconstruction)
           elbo = pxz_likelihood - kl_divergence # should be maximized
           loss = w_kl*kl_loss + w_r*recon_loss
           loss.backward()
           train_loss += loss.item()
```

```
train_kl_loss += kl_loss.item()
            train_recon_loss += recon_loss.item()
            train_kl_divergence += kl_divergence.item()
            train_pxz_likelihood += pxz_likelihood.item()
            train_elbo += elbo.item()
            optimizer.step()
        if use scheduler:
            scheduler.step()
       train_loss = train_loss/len(train_loader)
       train_kl_loss = train_kl_loss/len(train_loader)
       train_recon_loss = train_recon_loss/len(train_loader)
       train_kl_divergence = train_kl_divergence/len(train_loader)
       train_pxz_likelihood = train_pxz_likelihood/len(train_loader)
       train_elbo = train_elbo/len(train_loader)
       if (epoch<5) or (epoch\%5 == 0):
            print("Epoch {}, Loss {:.4f}, kl_loss {:.4f}, recon_loss {:.4f},__
→kl_divergence {:.4f}".format(epoch+1, float(train_loss),
→float(train kl loss), float(train recon loss), float(train kl divergence)))
             plot_latent(label, latent, dtype="tensor", suptitle_app="_train")
#
             plot_p_q(latent_mean, latent_logvar, suptitle_app="_train")
            if use_scheduler:
               print("current learning rate {}".format(scheduler.
→get_last_lr()))
            # test dataset, plot latent for one batch
           model.eval()
            for img, label in test loader:
                img, label = img.to(device), label.to(device)
                latent, reconstruction, latent mean, latent_logvar = model(img)
                plot_latent(label, latent, dtype="tensor", suptitle_app="_test")
               plot_p_q(latent_mean, latent_logvar, suptitle_app="_test")
                break
        epoch_train_loss.append(train_loss)
        epoch_train_kl_loss.append(train_kl_loss)
        epoch_train_recon_loss.append(train_recon_loss)
       epoch_sample_img.append(img.cpu().detach().numpy())
```

```
epoch_sample_reconstruction.append(reconstruction.cpu().detach().
       \rightarrownumpy())
              epoch_sample_latent.append(latent.cpu().detach().numpy())
              epoch_train_kl_divergence.append(train_kl_divergence)
              epoch train pxz likelihood.append(train pxz likelihood)
              epoch_train_elbo.append(train_elbo)
              results_dict = {
                  "train_loss": np.array(epoch_train_loss),
                  "train_kl_loss": np.array(epoch_train_kl_loss),
                  "train_recon_loss": np.array(epoch_train_recon_loss),
                  "sample_img": np.array(epoch_sample_img),
                  "sample_reconstruction": np.array(epoch_sample_reconstruction),
                  "sample_latent": np.array(epoch_sample_latent),
                  "train_kl_divergence": np.array(epoch_train_kl_divergence),
                  "train_pxz_likelihood": np.array(epoch_train_pxz_likelihood),
                  "train_elbo": np.array(epoch_train_elbo)
              }
          return model, results dict
 [9]: # use qpu if available
      device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
      input_shape = [1, 28, 28]
      enc dim = 400
      latent_dim = 2
      num epochs = 50
      learning_rate = 1e-3
      logDir = "models_and_stats/"
      w r = 1
      w kl = 10
      model_name = "MLP_VAE_dist_12_wkl_{}_wr_{}".format(w_kl, w_r)
      model_path = logDir + model_name + ".pt"
      dict_name = model_name + '.pkl'
[10]: pretrain = False
[11]: %%time
      if pretrain:
          # load the pretrained model
          model = MLP_VAE(input_shape=input_shape, enc_dim=enc_dim,__
       →latent_dim=latent_dim)
          model.load state dict(torch.load(model path))
          model.to(device)
          results_dict = pickle.load(open(logDir + dict_name, 'rb'))
```

```
else:
    # train and save the model
    for (w_kl, w_r) in [[1, 1]]: # [[10, 0], [10, 1]] # w_kl must be greater_
 \hookrightarrow than 0, otherwise kl_divergence easy to get nan
        model_name = "MLP_VAE_dist_12_wkl_{}_wr_{}".format(w_kl, w_r)
        model path = logDir + model name + ".pt"
        dict_name = model_name + '.pkl'
        model = MLP_VAE(input_shape=input_shape, enc_dim=enc_dim,__
 →latent_dim=latent_dim).to(device)
        model, results_dict = train(model, device, train_loader,__
 →num_epochs=num_epochs, learning_rate=learning_rate, use_scheduler=False,
 \hookrightarrow w_kl=w_kl, w_r=w_r)
        torch.save(model.state_dict(), model_path)
        pickle.dump(results_dict, open(logDir + dict_name, 'wb'))
        print("dump results dict to {}".format(dict_name))
model.eval()
```

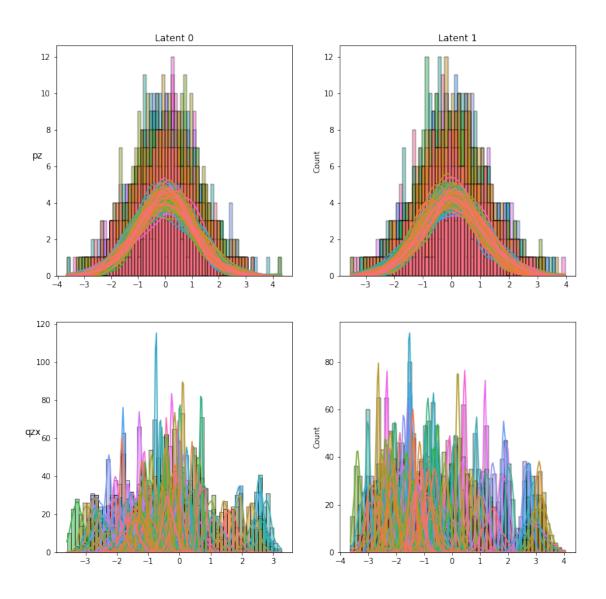
Epoch 1, Loss 24439.6577, kl_loss 741.7957, recon_loss 23697.8620, kl_divergence
629.5268
labels <class 'numpy.ndarray'> (128,)
latents <class 'numpy.ndarray'> (128, 2)

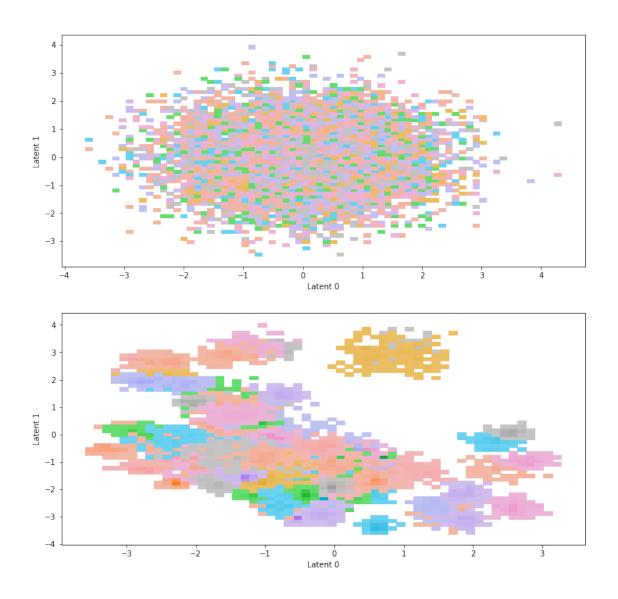


Plot bivariate latent distributions pz batch_shape torch.Size([128, 2]), event_shape torch.Size([])

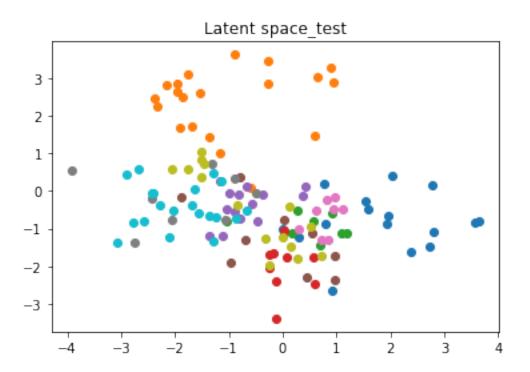
qzx batch_shape torch.Size([128, 2]), event_shape torch.Size([])
check p, q shape, pz (100, 128, 2), qzx (100, 128, 2)

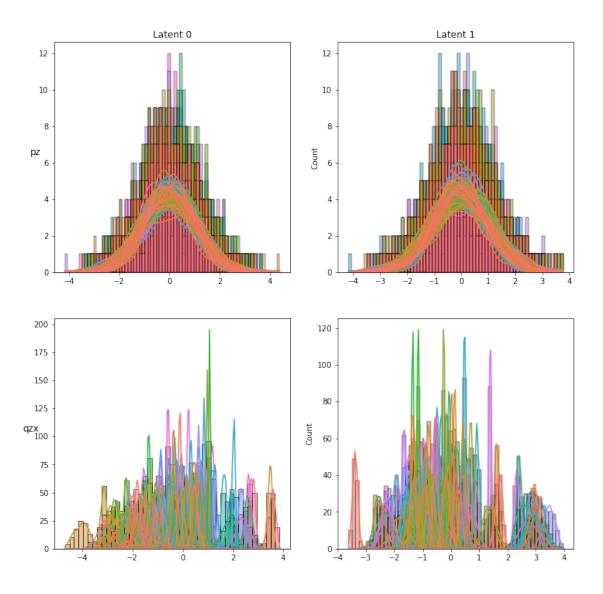
Bivariate Latent Distributions_test

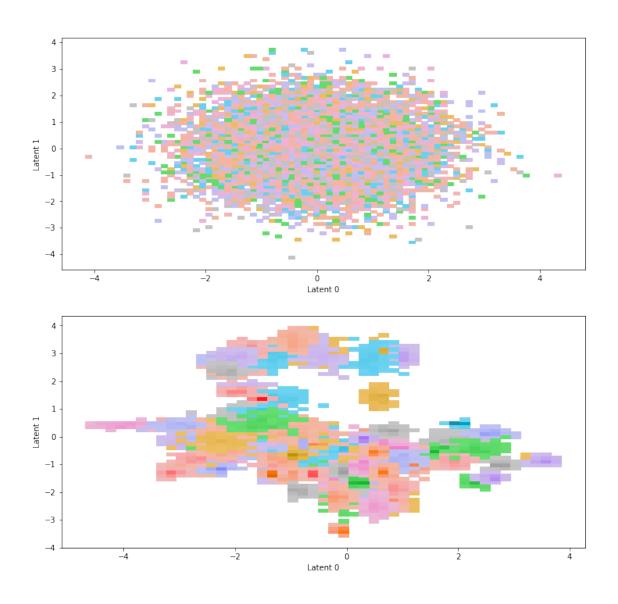




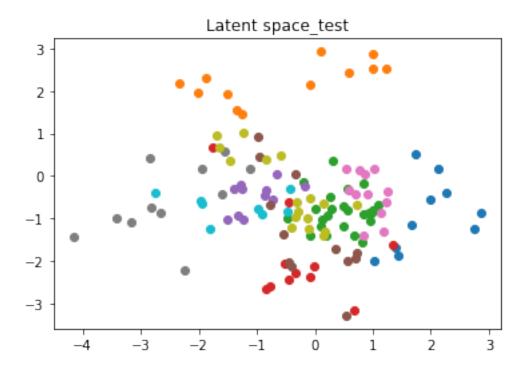
Epoch 2, Loss 21509.2626, kl_loss 672.1667, recon_loss 20837.0960, kl_divergence
491.2196
labels <class 'numpy.ndarray'> (128,)
latents <class 'numpy.ndarray'> (128, 2)

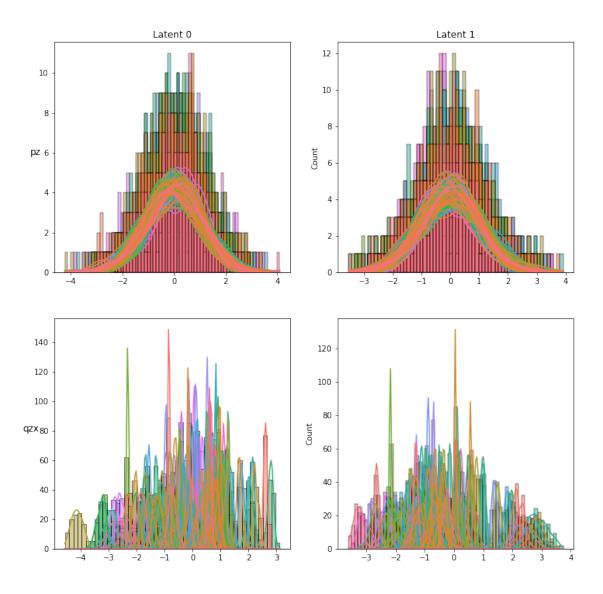


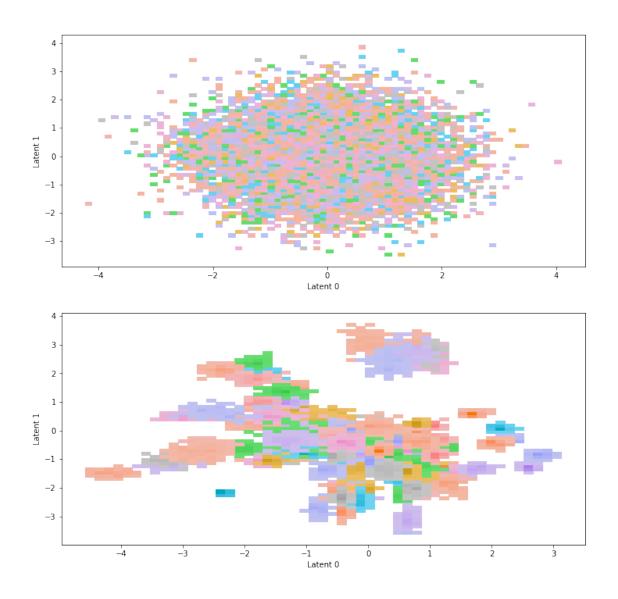




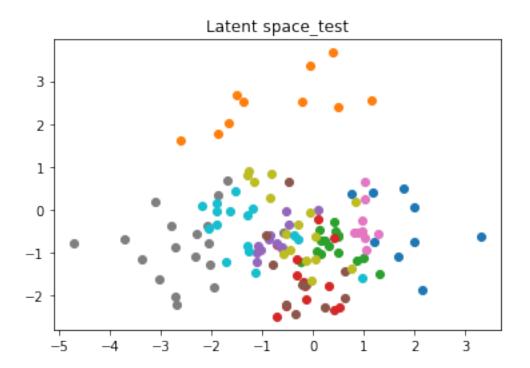
Epoch 3, Loss 20971.8730, kl_loss 686.6608, recon_loss 20285.2121, kl_divergence
470.0660
labels <class 'numpy.ndarray'> (128,)
latents <class 'numpy.ndarray'> (128, 2)

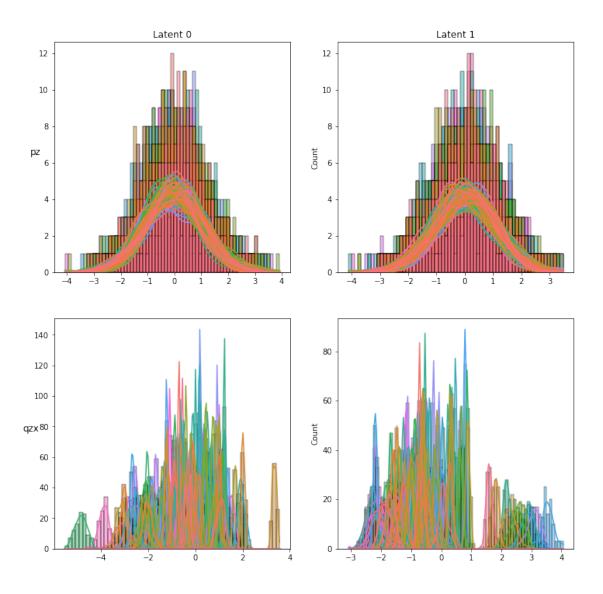


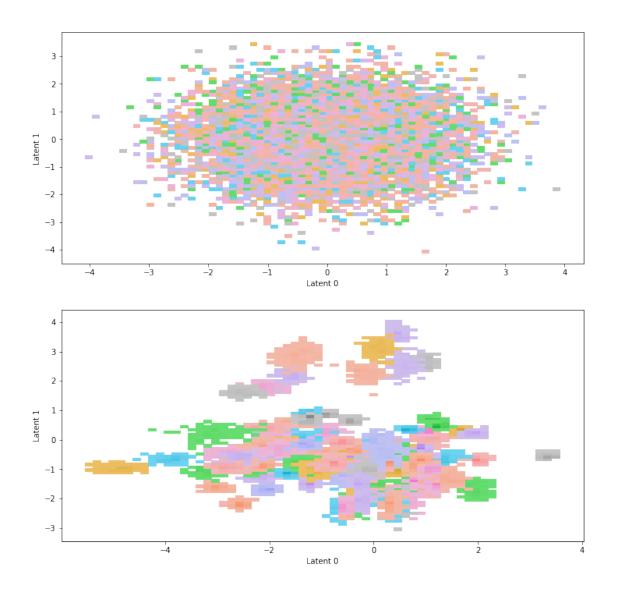




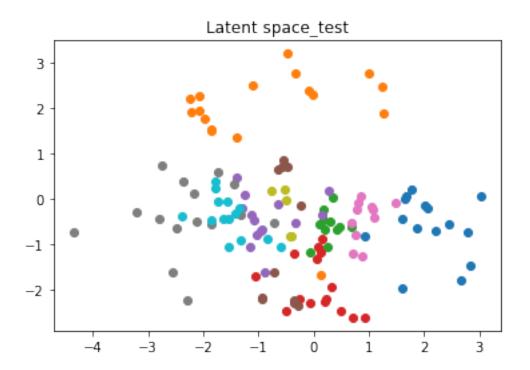
Epoch 4, Loss 20651.3581, kl_loss 696.2990, recon_loss 19955.0591, kl_divergence
459.3056
labels <class 'numpy.ndarray'> (128,)
latents <class 'numpy.ndarray'> (128, 2)

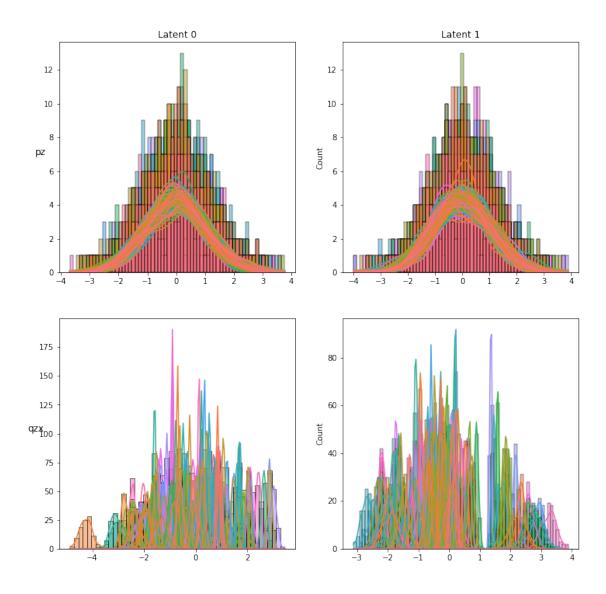


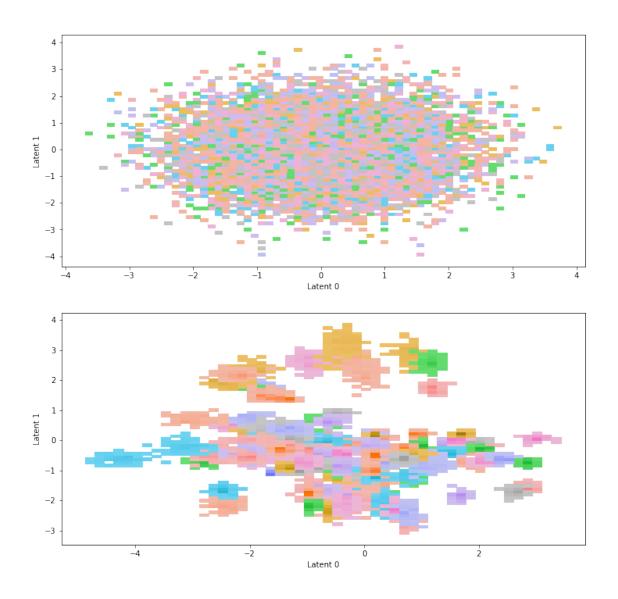




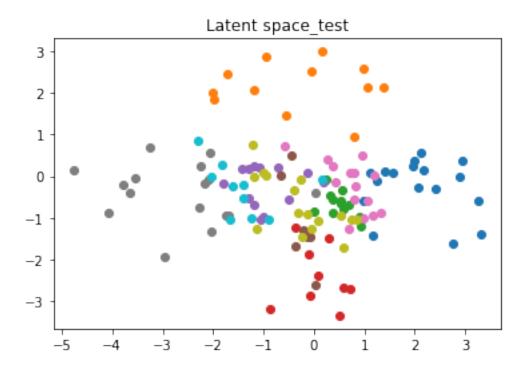
Epoch 5, Loss 20415.5679, kl_loss 704.8515, recon_loss 19710.7165, kl_divergence
452.7028
labels <class 'numpy.ndarray'> (128,)
latents <class 'numpy.ndarray'> (128, 2)

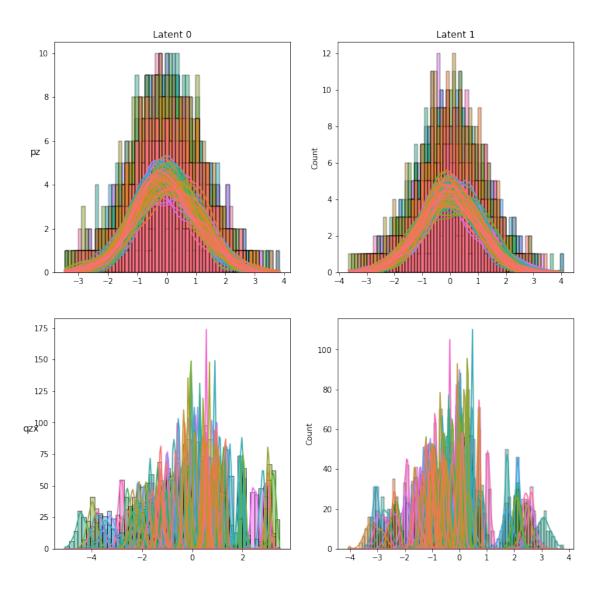


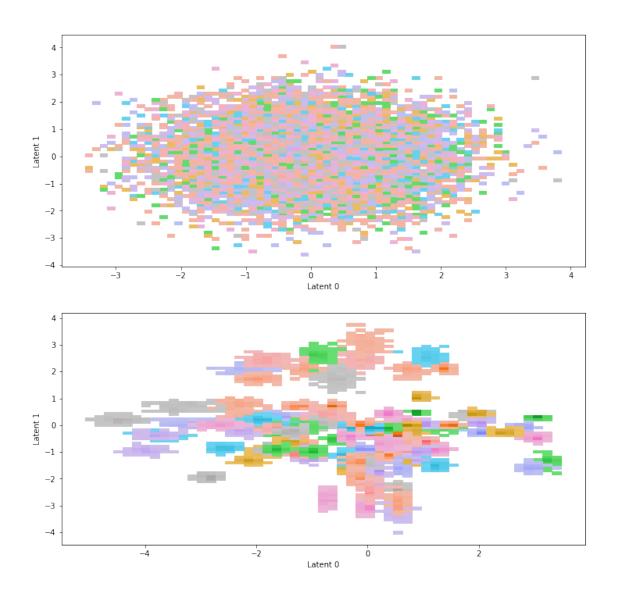




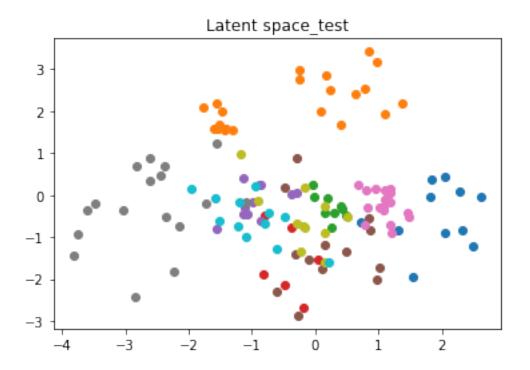
Epoch 6, Loss 20239.9587, kl_loss 713.9371, recon_loss 19526.0216, kl_divergence
449.2407
labels <class 'numpy.ndarray'> (128,)
latents <class 'numpy.ndarray'> (128, 2)

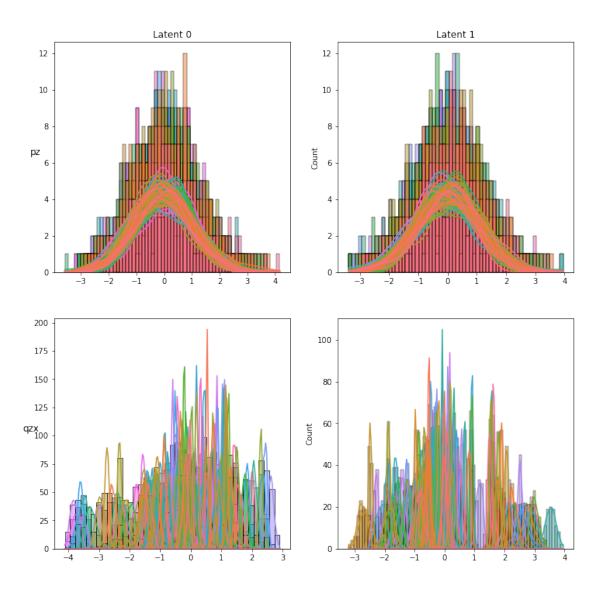


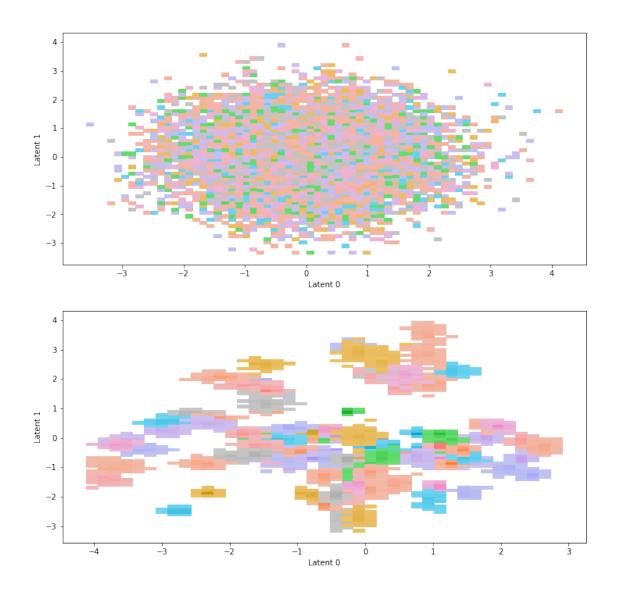




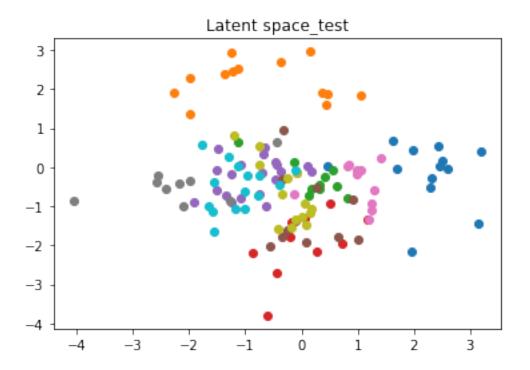
Epoch 11, Loss 19695.2986, kl_loss 745.8773, recon_loss 18949.4213,
kl_divergence 439.4040
labels <class 'numpy.ndarray'> (128,)
latents <class 'numpy.ndarray'> (128, 2)

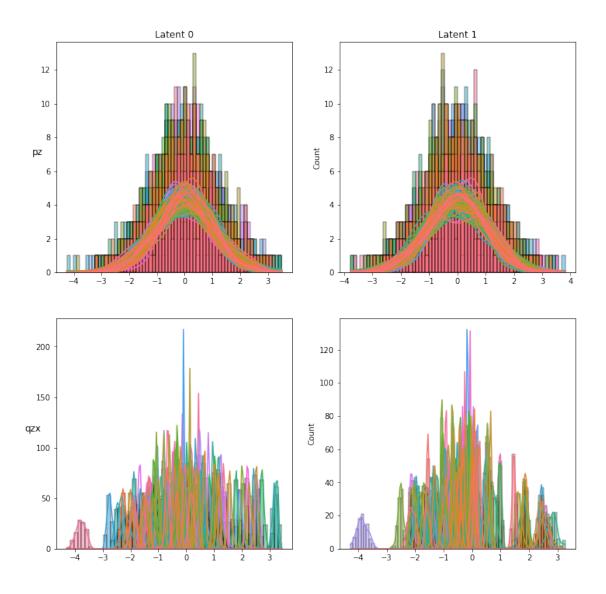


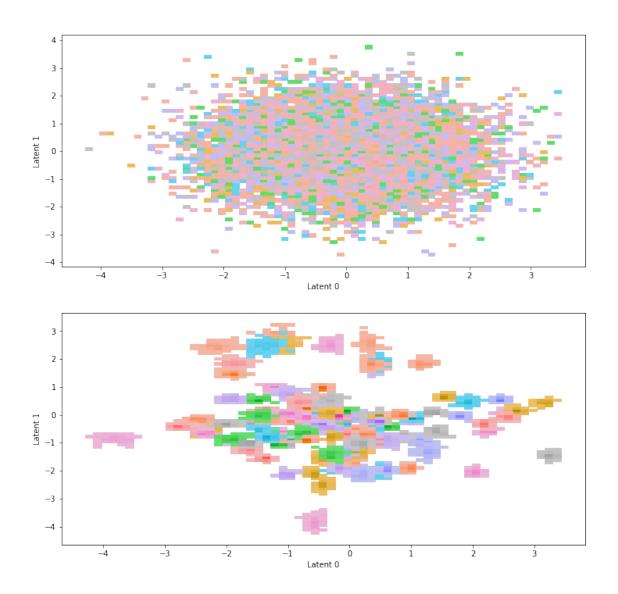




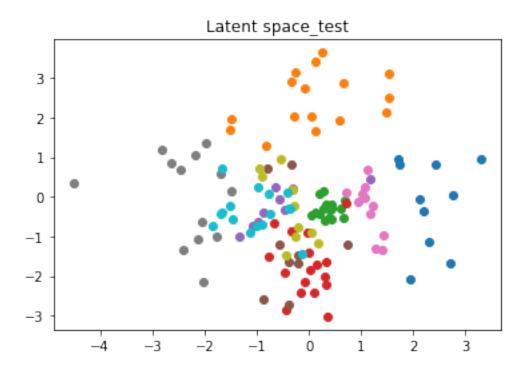
Epoch 16, Loss 19406.1731, kl_loss 763.7973, recon_loss 18642.3757,
kl_divergence 433.7580
labels <class 'numpy.ndarray'> (128,)
latents <class 'numpy.ndarray'> (128, 2)

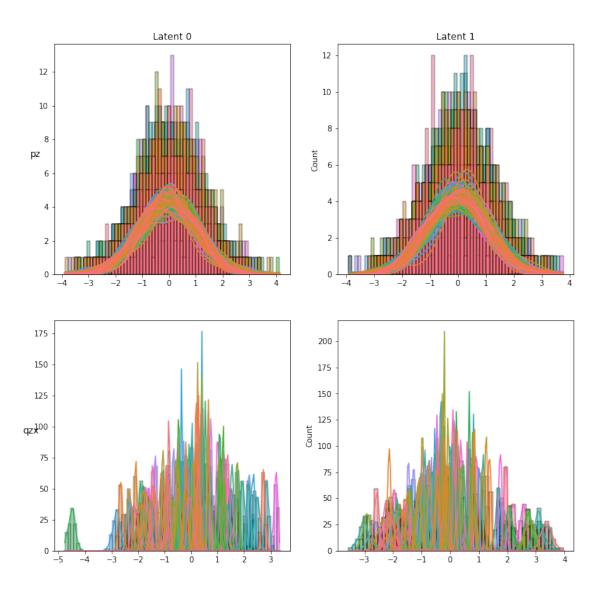


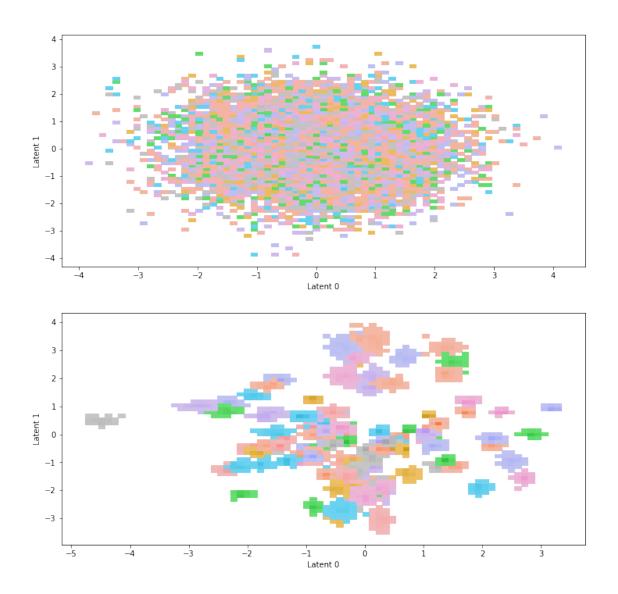




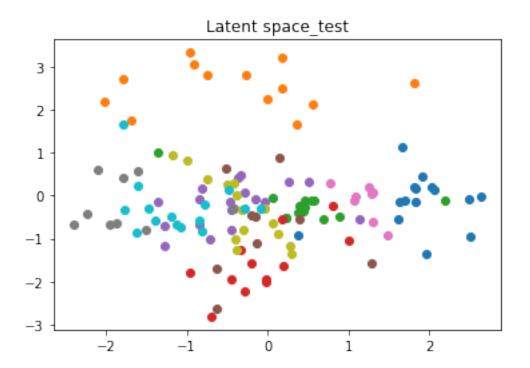
Epoch 21, Loss 19211.6567, kl_loss 777.7488, recon_loss 18433.9080,
kl_divergence 431.2480
labels <class 'numpy.ndarray'> (128,)
latents <class 'numpy.ndarray'> (128, 2)

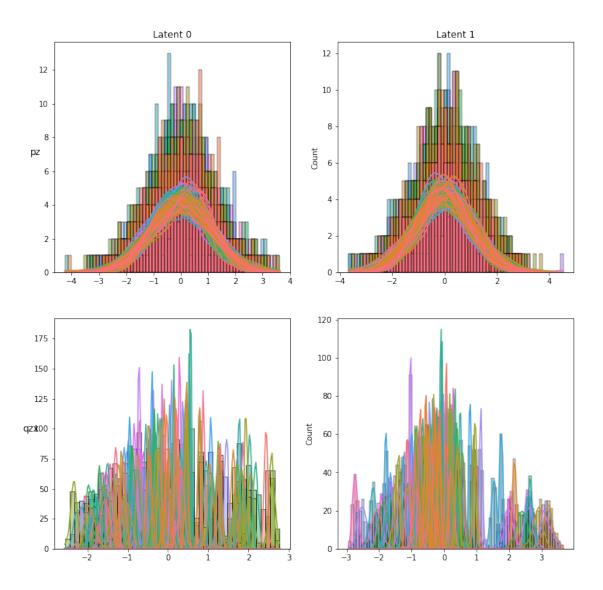


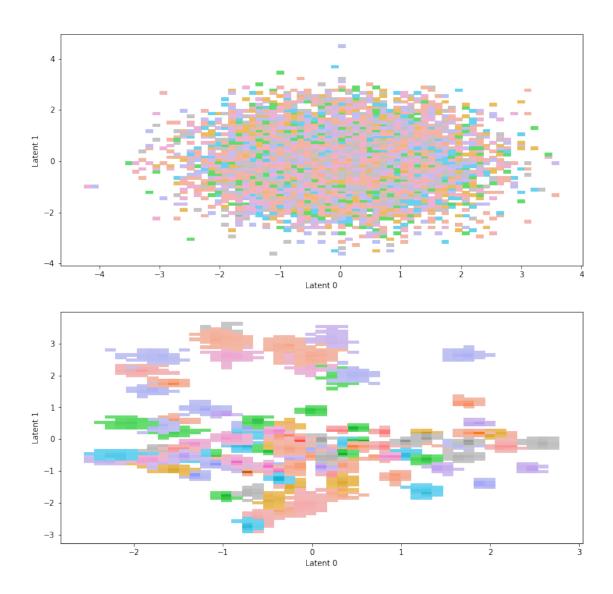




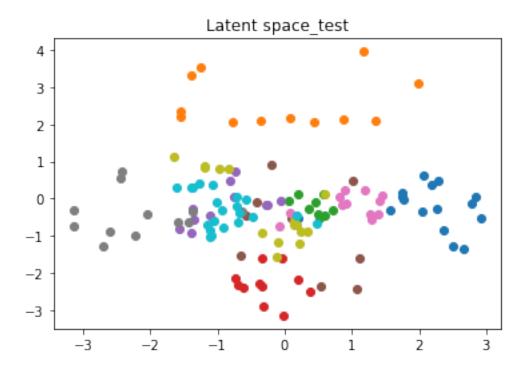
Epoch 26, Loss 19069.2299, kl_loss 788.0586, recon_loss 18281.1712,
kl_divergence 429.8770
labels <class 'numpy.ndarray'> (128,)
latents <class 'numpy.ndarray'> (128, 2)

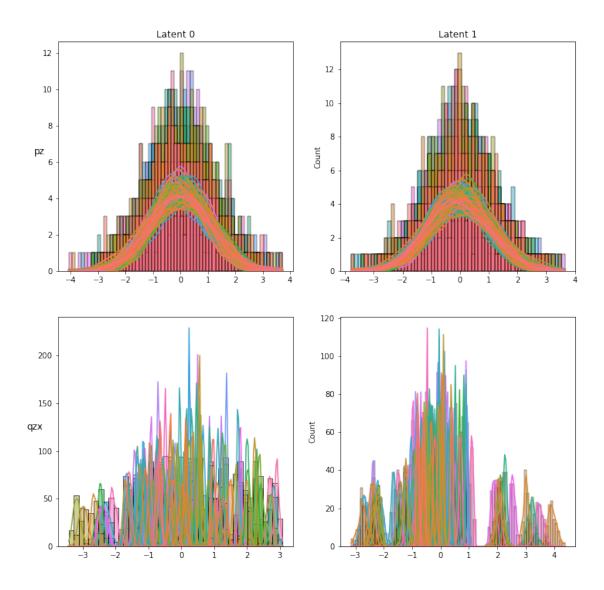


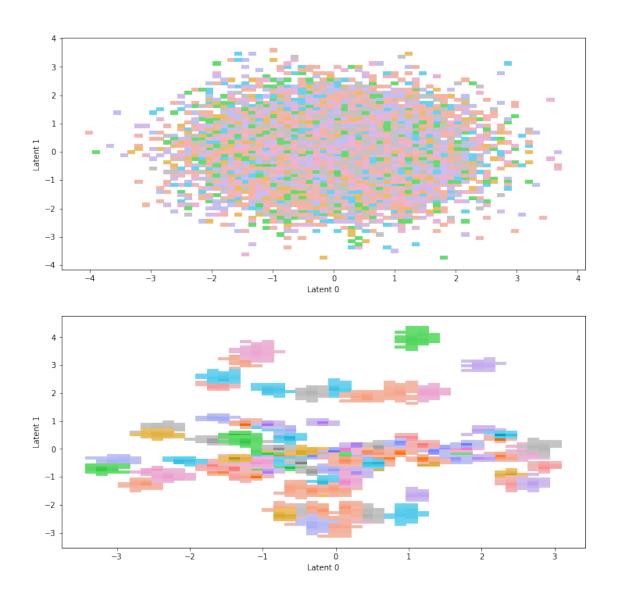




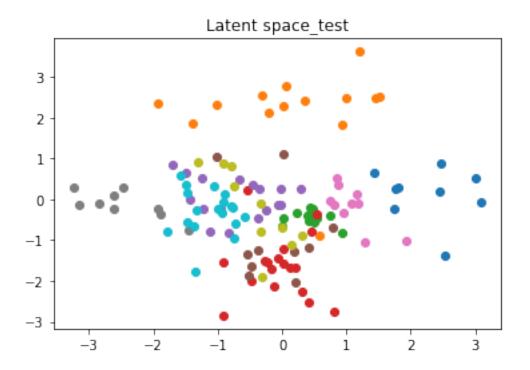
Epoch 31, Loss 18950.5296, kl_loss 796.8960, recon_loss 18153.6337,
kl_divergence 428.3900
labels <class 'numpy.ndarray'> (128,)
latents <class 'numpy.ndarray'> (128, 2)

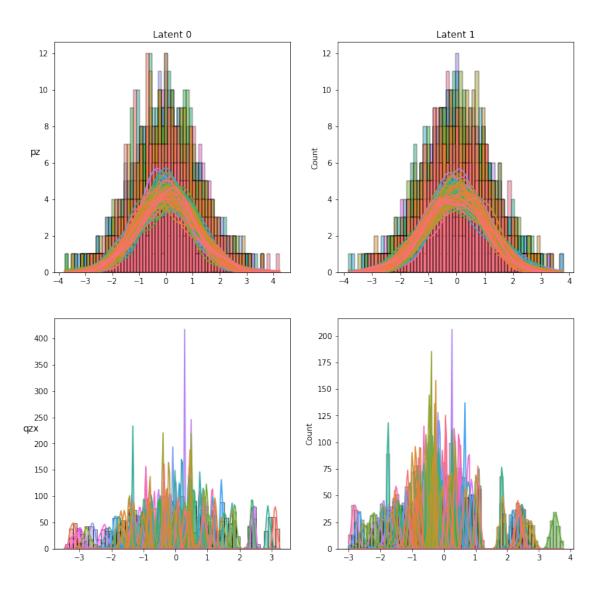


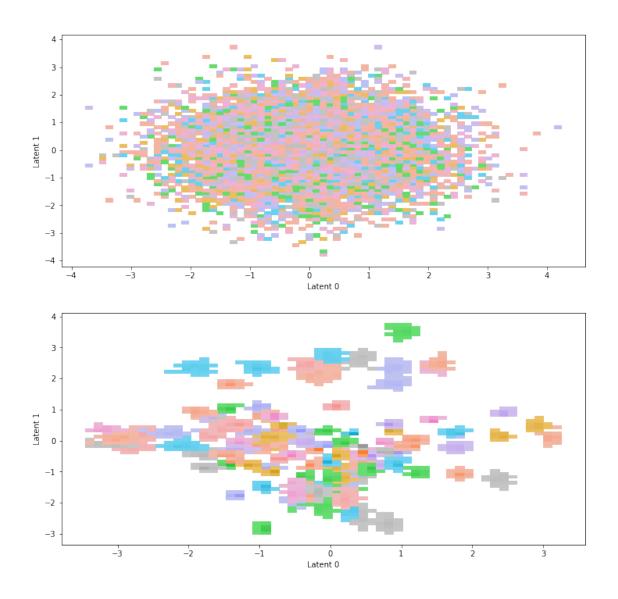




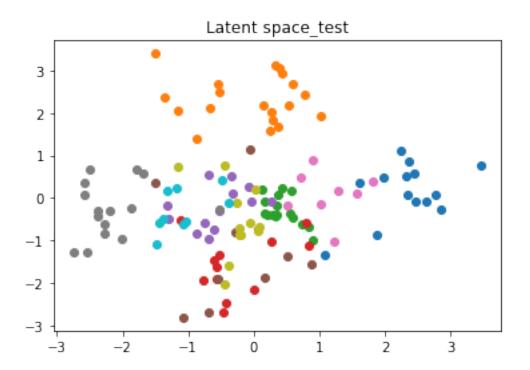
Epoch 36, Loss 18847.2089, kl_loss 803.6994, recon_loss 18043.5094,
kl_divergence 429.0268
labels <class 'numpy.ndarray'> (128,)
latents <class 'numpy.ndarray'> (128, 2)

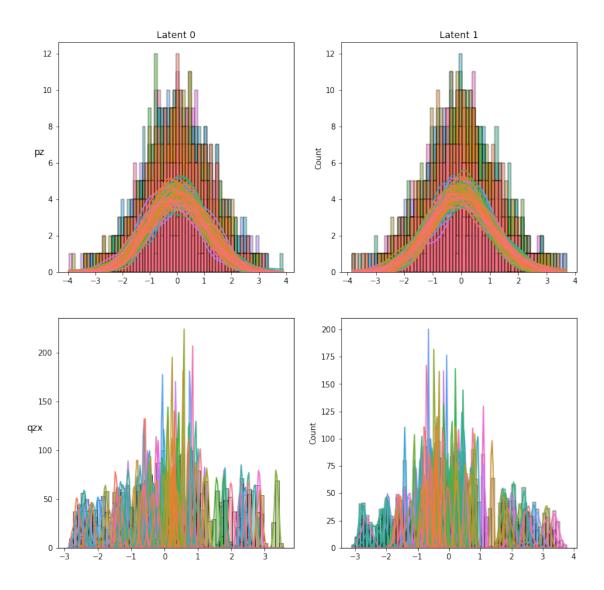


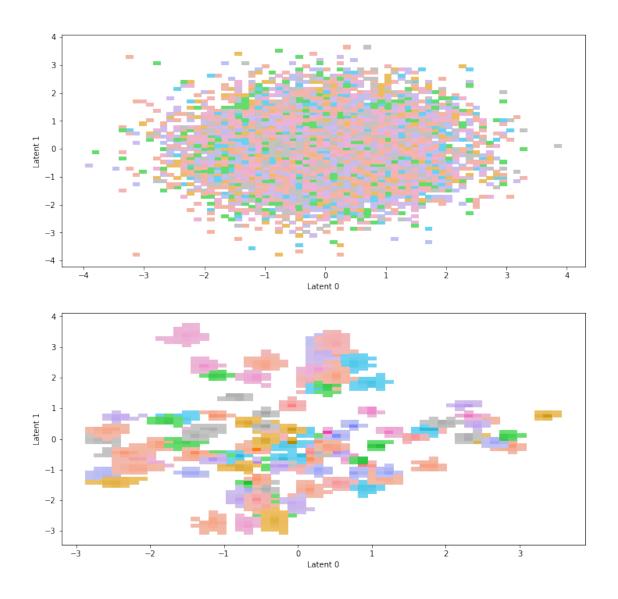




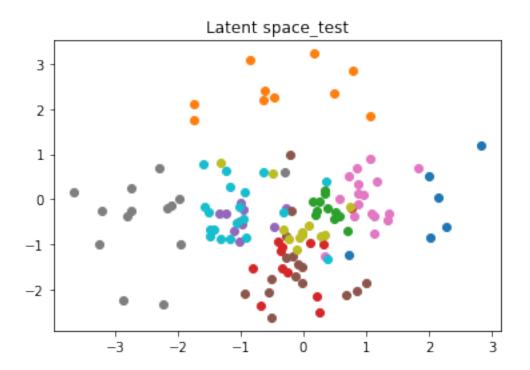
Epoch 41, Loss 18755.5544, kl_loss 806.9019, recon_loss 17948.6526,
kl_divergence 428.2860
labels <class 'numpy.ndarray'> (128,)
latents <class 'numpy.ndarray'> (128, 2)

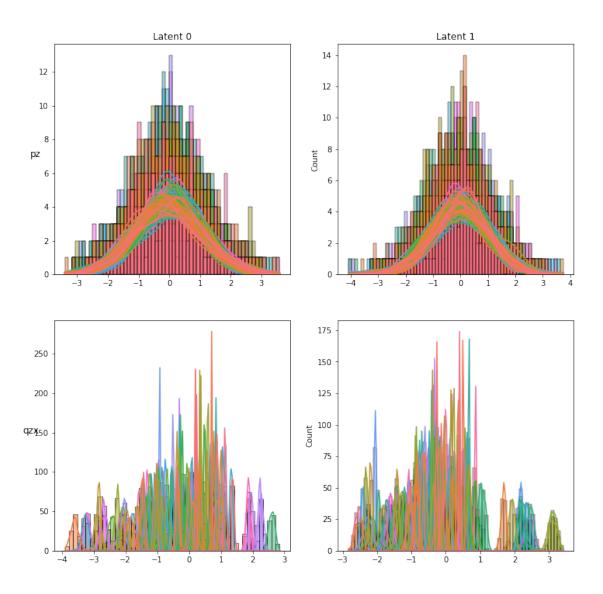


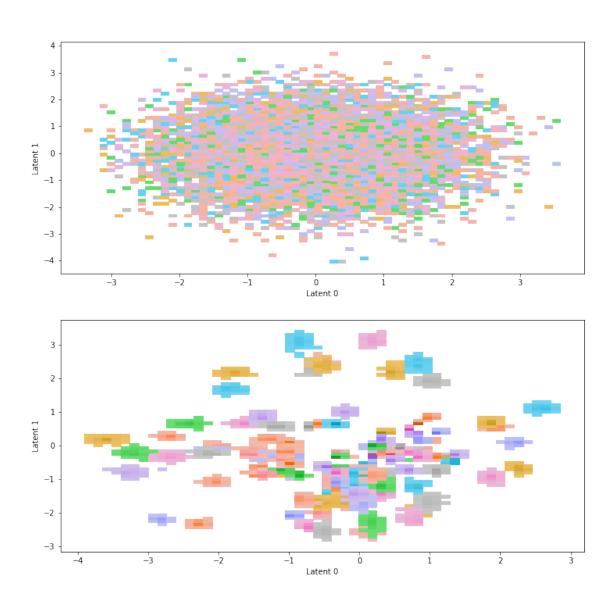




Epoch 46, Loss 18685.7947, kl_loss 813.6818, recon_loss 17872.1129,
kl_divergence 426.9016
labels <class 'numpy.ndarray'> (128,)
latents <class 'numpy.ndarray'> (128, 2)





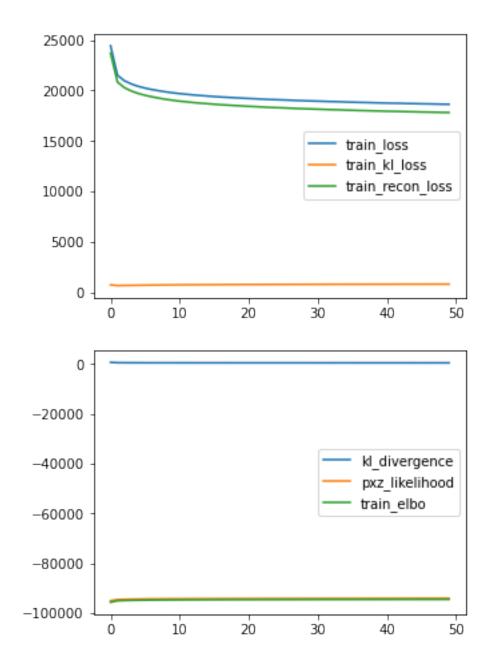


```
(decoder): MLP_V_Decoder(
    (model): Sequential(
        (0): Linear(in_features=2, out_features=400, bias=True)
        (1): ReLU()
        (2): Linear(in_features=400, out_features=784, bias=True)
        (3): Sigmoid()
    )
)
(enc_to_mean): Linear(in_features=400, out_features=2, bias=True)
    (enc_to_logvar): Linear(in_features=400, out_features=2, bias=True)
)
```

3.4 Visualization of the training process and results

3.4.1 plot the learning curve

```
[12]: epoch_train_loss = results_dict["train_loss"]
      epoch_train_kl_loss = results_dict["train_kl_loss"]
      epoch_train_recon_loss = results_dict["train_recon_loss"]
      epoch_train_kl_divergence = results_dict["train_kl_divergence"]
      epoch_train_pxz_likelihood = results_dict["train_pxz_likelihood"]
      epoch_train_elbo = results_dict["train_elbo"]
      fig, axes = plt.subplots(2,1, figsize=(5,8))
      assert len(epoch_train_loss)==num_epochs, "check num_epochs"
      axes[0].plot(np.arange(num_epochs), epoch_train_loss, label="train_loss")
      axes[0].plot(np.arange(num epochs), epoch train kl loss, label="train kl loss")
      axes[0].plot(np.arange(num_epochs), epoch_train_recon_loss,_
       →label="train recon loss")
      axes[0].legend()
      axes[1].plot(np.arange(num_epochs), epoch_train_kl_divergence,_
       →label="kl_divergence")
      axes[1].plot(np.arange(num_epochs), epoch_train_pxz_likelihood,__
      →label="pxz_likelihood")
      axes[1].plot(np.arange(num_epochs), epoch_train_elbo, label="train_elbo")
      axes[1].legend()
      plt.show()
```

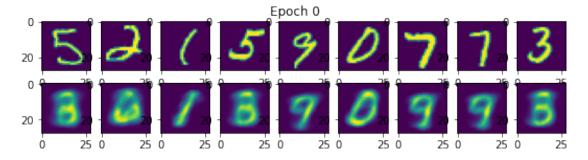


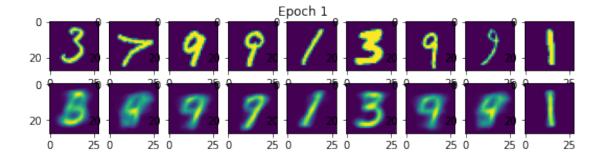
3.4.2 plot the evolution of reconstruction through epochs

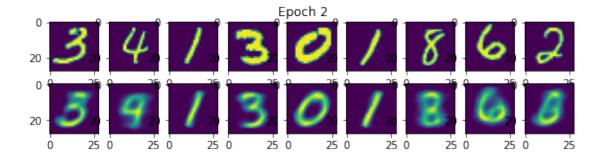
```
[13]: num_cols = 9
selected_epochs = np.concatenate((np.arange(5),np.arange(10,num_epochs,10)))
for epoch in selected_epochs:
    figure = plt.figure(figsize=(num_cols,2))
    figure.suptitle("Epoch {}".format(epoch))
    imgs = results_dict["sample_img"][epoch]
```

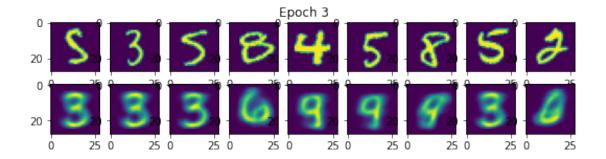
```
reconstructions = results_dict["sample_reconstruction"][epoch]
for i, item in enumerate(imgs):
    # plot only first few images
    if i>=num_cols: break
    plt.subplot(2,num_cols, i+1)
    plt.imshow(item[0])

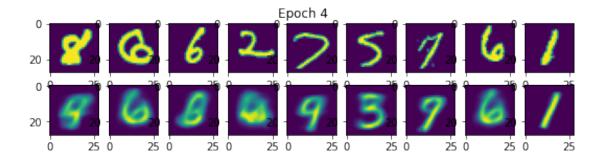
for i, item in enumerate(reconstructions):
    if i>=num_cols: break
    plt.subplot(2, num_cols, num_cols+i+1)
    plt.imshow(item[0])
```

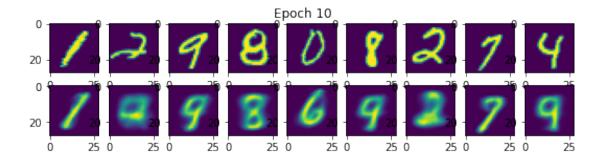


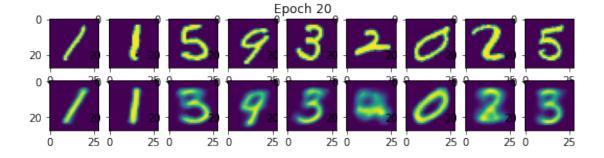


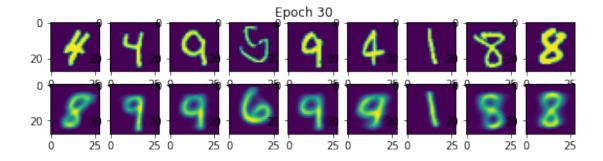


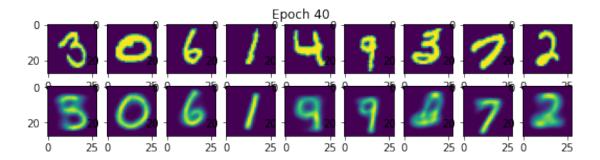












3.4.3 plot the latent space

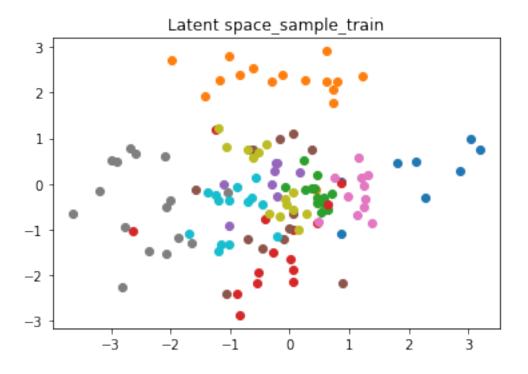
The hover part takes reference from this post

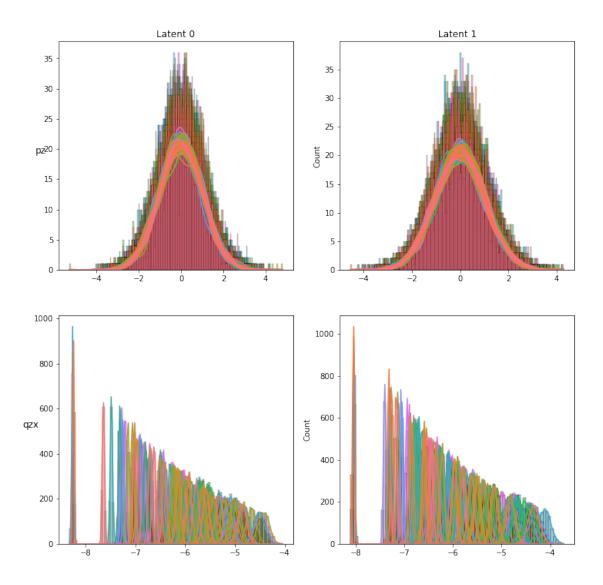
```
model.eval()
sample_train_imgs, sample_train_labels = next(iter(train_loader))
print(sample_train_imgs.shape, sample_train_labels.shape)
sample_test_imgs, sample_test_labels = next(iter(test_loader))
print(sample_test_imgs.shape, sample_test_labels.shape)
sample_train_imgs, sample_test_imgs = torch.tensor(sample_train_imgs).float().

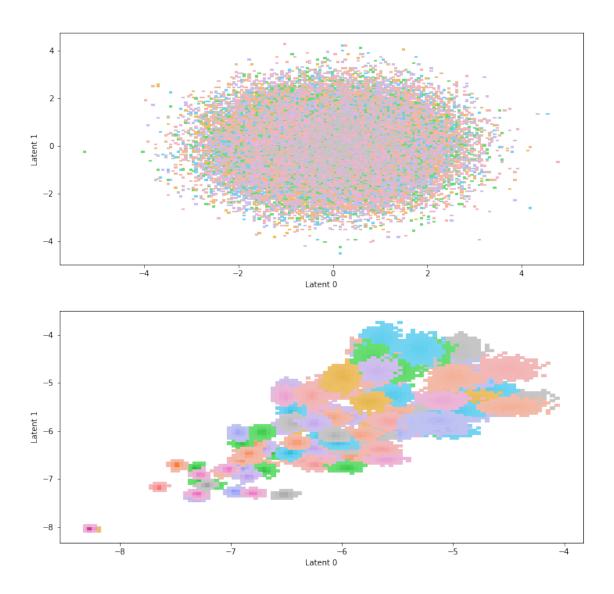
to(device), torch.tensor(sample_test_imgs).float().to(device)
```

```
torch.Size([128, 1, 28, 28]) torch.Size([128]) torch.Size([128, 1, 28, 28]) torch.Size([128])
```

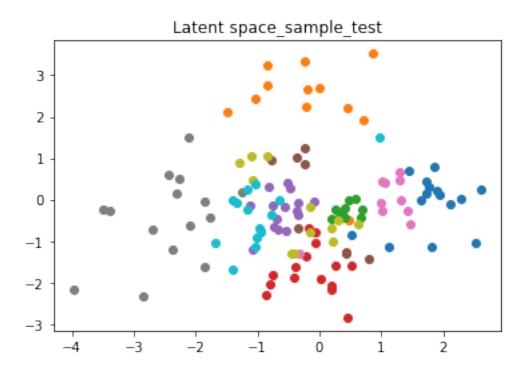
labels <class 'numpy.ndarray'> (128,)
latents <class 'numpy.ndarray'> (128, 2)

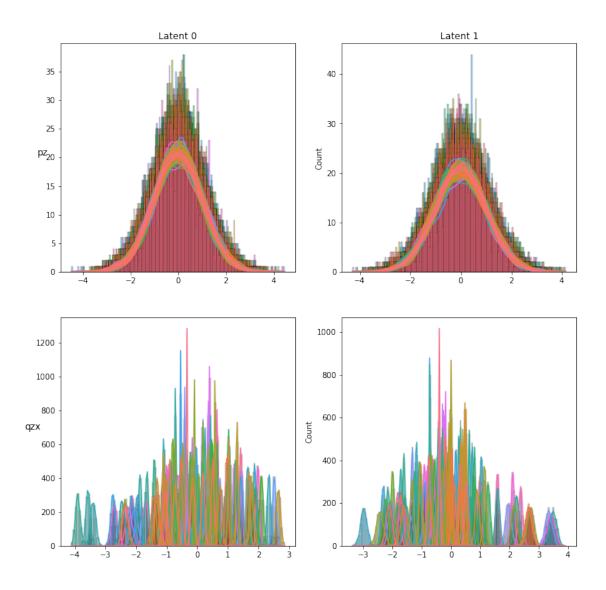


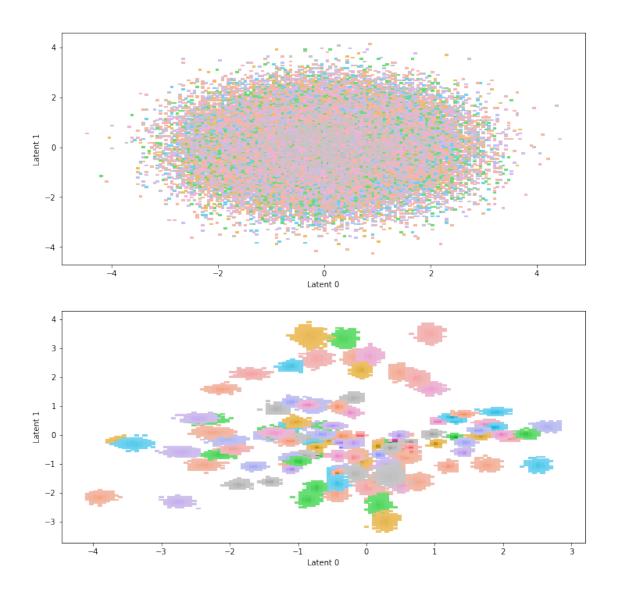




labels <class 'numpy.ndarray'> (128,)
latents <class 'numpy.ndarray'> (128, 2)

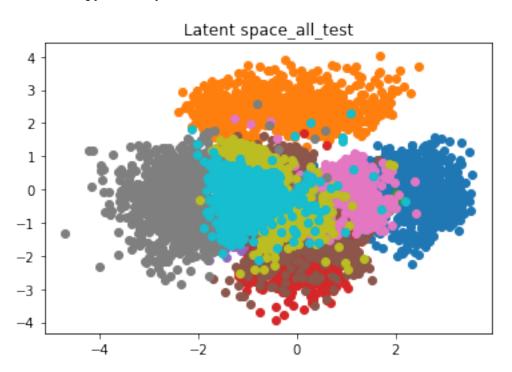






```
# plot_p_q(all_test_latent_means, all_test_latent_logvars, N_samples=1000, U_sample_test_s) # U_sample_test_s + U_sample_test_s # U_sample_test_s + U_sample_test_s
```

```
labels <class 'numpy.ndarray'> (10000,)
latents <class 'numpy.ndarray'> (10000, 2)
```



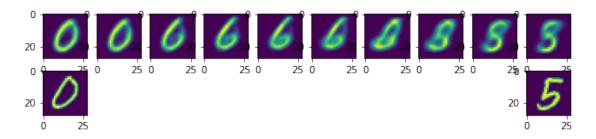
```
[17]: all_test_latents = all_test_latents.cpu().detach().numpy()
all_test_labels = all_test_labels.cpu().detach().numpy()
```

3.4.4 Interpolation between any two images

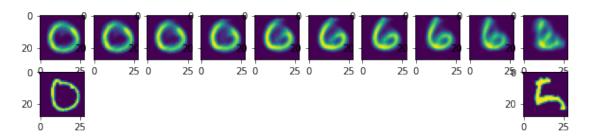
```
[19]: %matplotlib inline
[20]: def interpolate(index1, index2):
          x1 = results_dict["sample_img"][-1][index1]
          x2 = results_dict["sample_img"][-1][index2]
          x1, x2 = torch.from_numpy(x1).float().to(device), torch.from_numpy(x2).
       →float().to(device)
          x = torch.stack([x1, x2])
          latent_mean, latent_logvar = model.encode(x)
          embedding = model.sample_latent_embedding(latent_mean, latent_logvar)
          e1 = embedding[0]
          e2 = embedding[1]
          embedding_values = []
          for i in range(10):
              e = e1 * (i/10) + e2 * (10-i)/10
              embedding_values.append(e)
          embedding_values = torch.stack(embedding_values)
          recon_from_embeddings = model.decoder(embedding_values) # shape [10, 1, 28, ]
       <del>→</del>28]
          plt.figure(figsize=(10,2))
          for i, recon in enumerate(recon_from_embeddings.cpu().detach().numpy()):
              plt.subplot(2, 10, i+1)
              plt.imshow(recon[0])
```

```
# plot two original images
plt.subplot(2, 10, 11)
plt.imshow(x2.cpu().detach().numpy()[0])
plt.subplot(2, 10, 20)
plt.imshow(x1.cpu().detach().numpy()[0])
```

[21]: interpolate(3,5)



[22]: interpolate(2,7)



3.4.5 Interactive scroll bar for latent space

see VAE_MNIST_Interactive_ScrollBar