CVAE_dist_MNIST_StaticPlot

March 26, 2021

1 MLP Conditional 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
```

[4]:
```
batch_size = 128

transform = torchvision.transforms.Compose([torchvision.transforms.ToTensor()])

train_dataset = torchvision.datasets.MNIST(
    root="../data/", train=True, transform=transform, download=True)
train_loader = torch.utils.data.DataLoader(train_dataset,␣
↪batch_size=batch_size, shuffle=True)

test_dataset = torchvision.datasets.MNIST(
    root="../data/", train=False, transform=transform, download=True)
test_loader = torch.utils.data.DataLoader(test_dataset, batch_size=batch_size,␣
↪shuffle=True)
```

3.2 Conditional Variational Autoencoder

A MLP conditional variational autoencoder is used. Problem of VAE: we cannot control what kind of data is generatedl Based on the VAE, add conditions c at both input and latent space, so that true prior $p(z)$ becomes $p(z|c)$, approximated posterior $q(z|x)$ becomes $q(z|x,c)$ The condition c actually can be anything. Here it is implemented as ground truch label y

[5]:
```
class MLP_CV_Encoder(nn.Module):
    def __init__(self, **kwargs):
        super(MLP_CV_Encoder, self).__init__()

        self.model = nn.Sequential(
            nn.Linear(in_features=(np.prod(kwargs["input_shape"])+1),␣
↪out_features=kwargs["enc_dim"]),
            nn.ReLU(),
#              nn.Linear(in_features=400, out_features=kwargs["enc_dim"]),
#              nn.ReLU(),
        )


    def forward(self, x, y):
        y = torch.unsqueeze(y,1)
        x = torch.flatten(x, start_dim=1)
        x = torch.cat([x, y], dim = 1)
        enc_out = self.model(x)
        return enc_out
```

[6]:
```
class MLP_CV_Decoder(nn.Module):
    def __init__(self, **kwargs):
        super(MLP_CV_Decoder, self).__init__()
        self.model = nn.Sequential(
            nn.Linear(in_features=(kwargs["latent_dim"]+1),␣
↪out_features=kwargs["enc_dim"]),
            nn.ReLU(),
            nn.Linear(in_features=kwargs["enc_dim"], out_features=np.
↪prod(kwargs["input_shape"])),
            nn.Sigmoid() # push the pixels in range (0,1)
        )
        self.output_shape = kwargs["input_shape"]

    def forward(self, latent, y):
        y = torch.unsqueeze(y,1)
        latent = torch.cat([latent, y], dim=1)
        x_bar = self.model(latent)
        x_bar = x_bar.view([-1]+ self.output_shape)
        return x_bar
```

[7]:
```
class MLP_CVAE(nn.Module):
    """
    TODO: check whether to use sum or mean for the probability part
    """
    def __init__(self, **kwargs):
        # kwargs["input_shape"] = [1,28,28]
        # kwargs["latent_dim"] = 4
        super(MLP_CVAE, self).__init__()
        self.encoder = MLP_CV_Encoder(**kwargs)
        self.decoder = MLP_CV_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, y):
        enc_out = self.encoder(x, y)
        mean = self.enc_to_mean(enc_out)
        logvar = self.enc_to_logvar(enc_out)
        return mean, logvar

    def decode(self, latent, y):
        return self.decoder(latent, y)

    def pxz_likelihood(self, x, x_bar, scale=1., dist_type="Gaussian"):
```

```
        """
        compute the likelihood p(x|z) based on predefined distribution, given a 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␣
↪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, y, if_plot_pq=False):
        latent_mean, latent_logvar = self.encode(x, y)
        latent = self.reparameterize(latent_mean, latent_logvar)
        x_bar = self.decoder(latent, y)

        if if_plot_pq:
            plot_p_q(latent_mean, latent_logvar)

        return latent, x_bar, latent_mean, latent_logvar
```

3.3 Training process

[8]:
```
def train(model, device, train_loader, num_epochs=5, learning_rate=1e-3,␣
↪use_scheduler=False, w_kl=10, w_r=1):
    recon_loss_fn = nn.BCELoss(reduction="sum")

    optimizer = optim.Adam(model.parameters(),
                           lr=learning_rate,
                            # weight_decay=5e-4,
                            )
    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,␣
↪label)
```

```
            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,␣
↪label)
#                 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().
↪numpy())
        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
```

[22]:
```
# use gpu 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_l2_wkl_{}_wr_{}".format(w_kl, w_r)
model_path = logDir + model_name + ".pt"
```

```
dict_name = model_name + '.pkl'
```

[23]:
```
pretrain = True
```

[24]:
```
%%time
if pretrain:
    # load the pretrained model
    model = MLP_CVAE(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 in [10]: # 1
        model_name = "MLP_VAE_dist_l2_wkl_{}_wr_{}".format(w_kl, w_r)
        model_path = logDir + model_name + ".pt"
        dict_name = model_name + '.pkl'
        model = MLP_CVAE(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,␣
 ↪w_kl=w_kl)
        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()
```

```
CPU times: user 9.62 ms, sys: 20.1 ms, total: 29.7 ms
Wall time: 29.4 ms
```

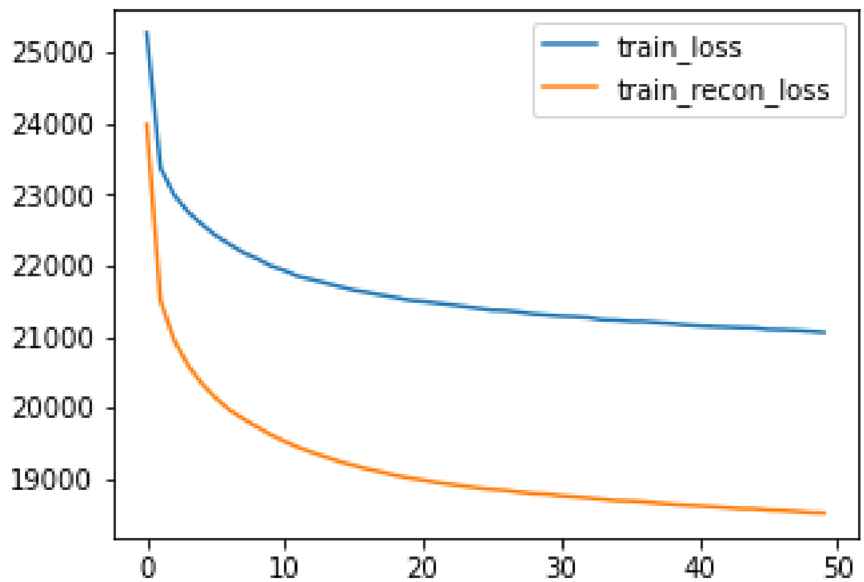
[24]:
```
MLP_CVAE(
  (encoder): MLP_CV_Encoder(
    (model): Sequential(
      (0): Linear(in_features=785, out_features=400, bias=True)
      (1): ReLU()
    )
  )
  (decoder): MLP_CV_Decoder(
    (model): Sequential(
      (0): Linear(in_features=3, out_features=400, bias=True)
      (1): ReLU()
      (2): Linear(in_features=400, out_features=784, bias=True)
      (3): Sigmoid()
    )
```

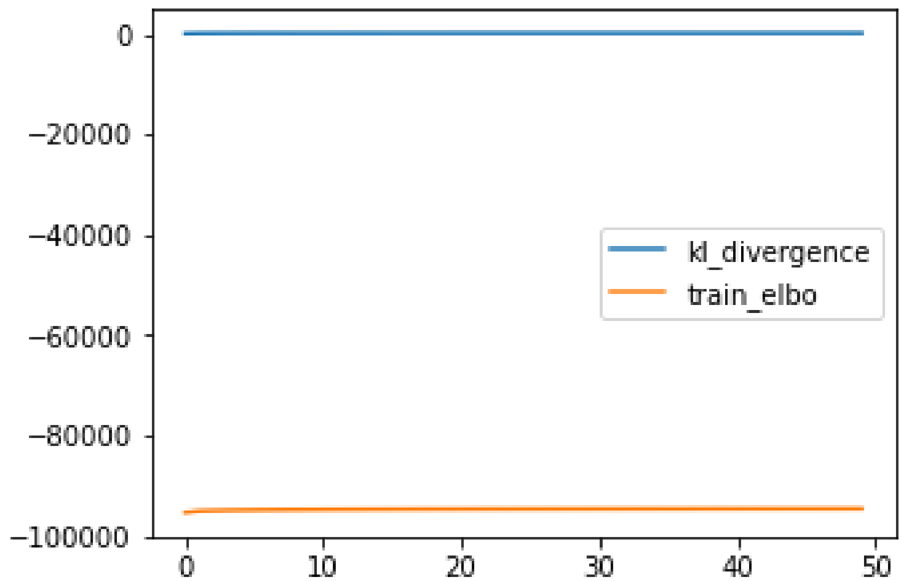
```
  )
  (enc_to_mean): Linear(in_features=400, out_features=2, bias=True)
  (enc_to_logvar): Linear(in_features=400, out_features=2, bias=True)
)
```

3.4 Visualization of the training process and results

3.4.1 plot the learning curve

[25]:
```
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()
```

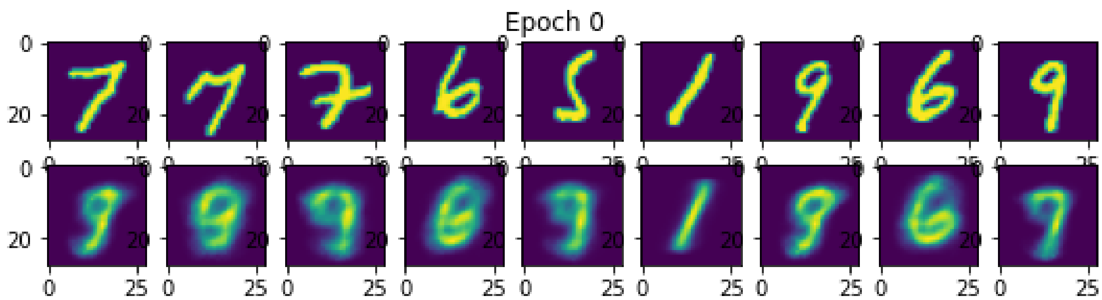


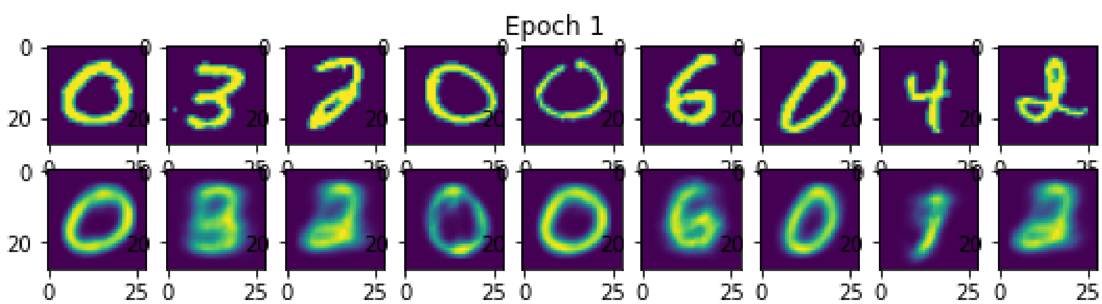


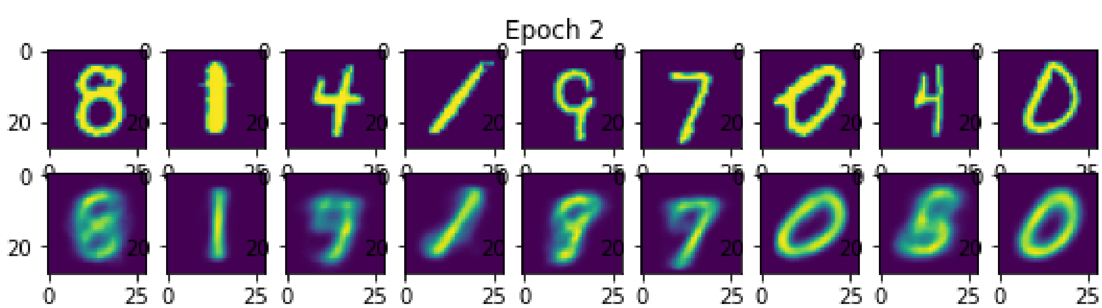
3.4.2 plot the evolution of reconstruction through epochs

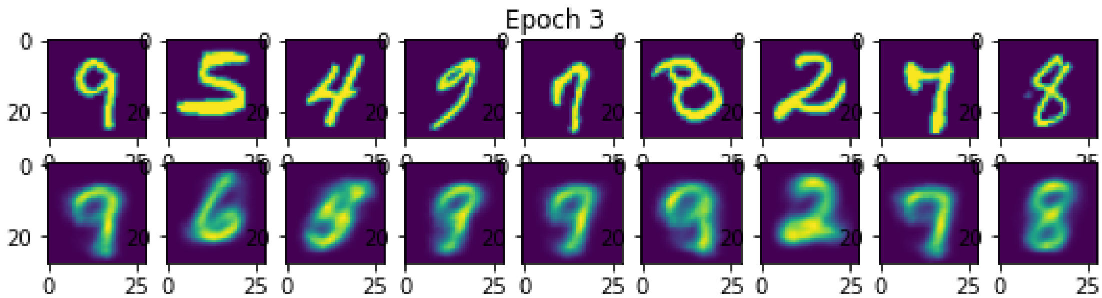
[26]:
```
num_cols = 9
selected_epochs = np.concatenate((np.arange(5),np.arange(10,num_epochs,10)))
for epoch in selected_epochs:
    figure = plt.figure(figsize=(num_cols,2))
    figure.suptitle("Epoch {}".format(epoch))
    imgs = results_dict["sample_img"][epoch]
```

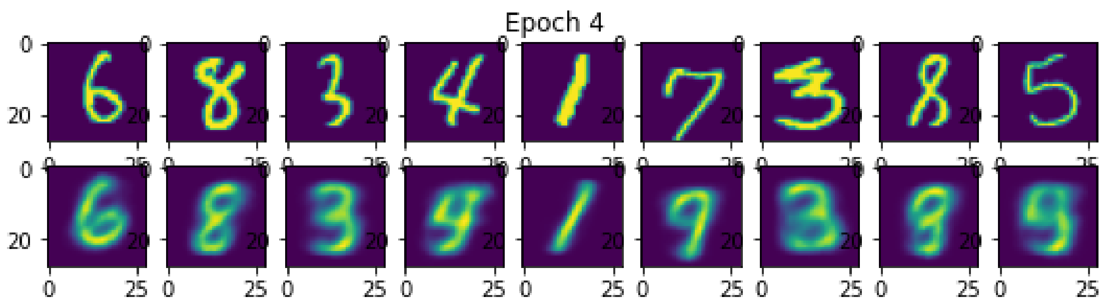
```
reconstructions = results_dict["sample_reconstruction"][epoch]
for i, item in enumerate(imgs):
    # plot only first few images
    if i>=num_cols: break
    plt.subplot(2,num_cols, i+1)
    plt.imshow(item[0])

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

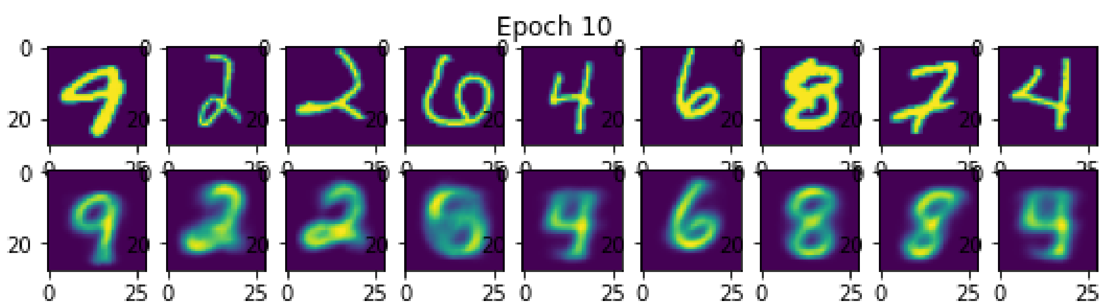


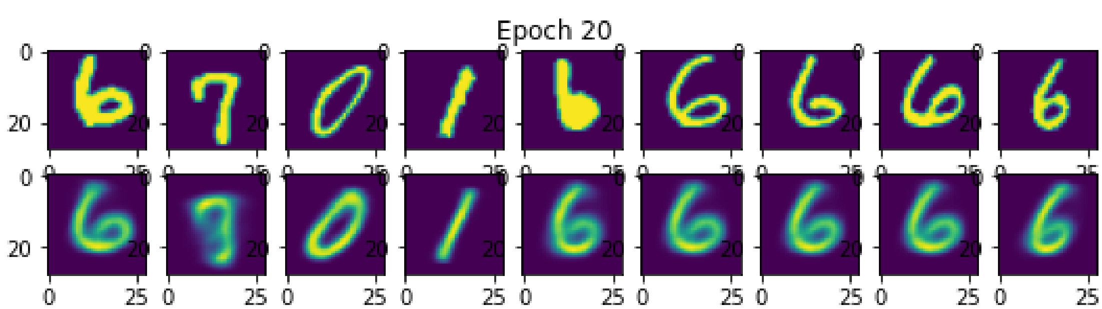


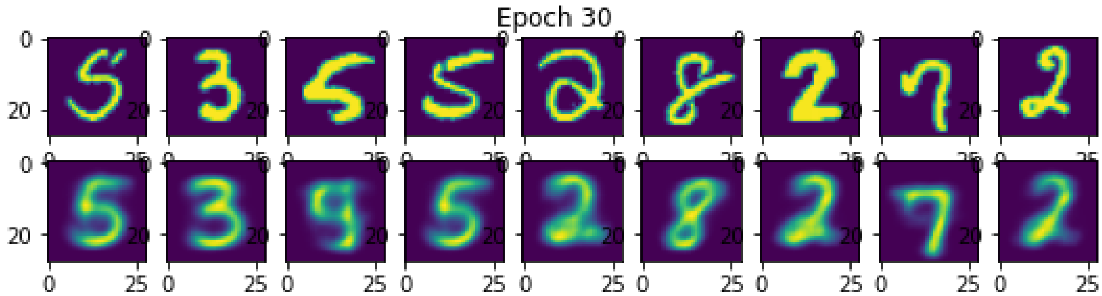


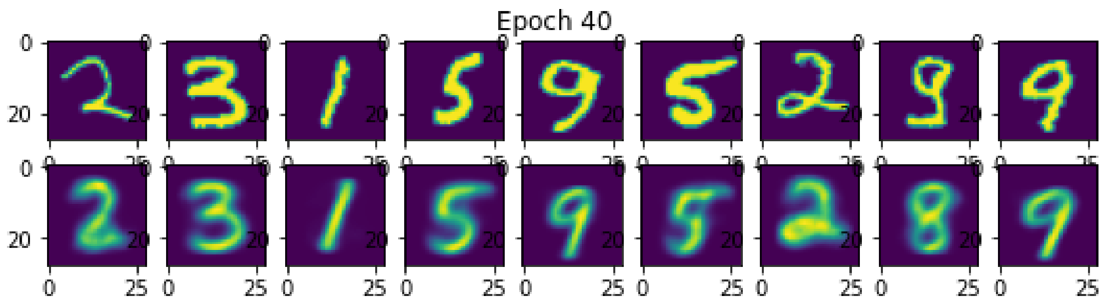

Epoch 3


Epoch 4


Epoch 10


Epoch 20





3.4.3 plot the latent space

The hover part takes reference from this post

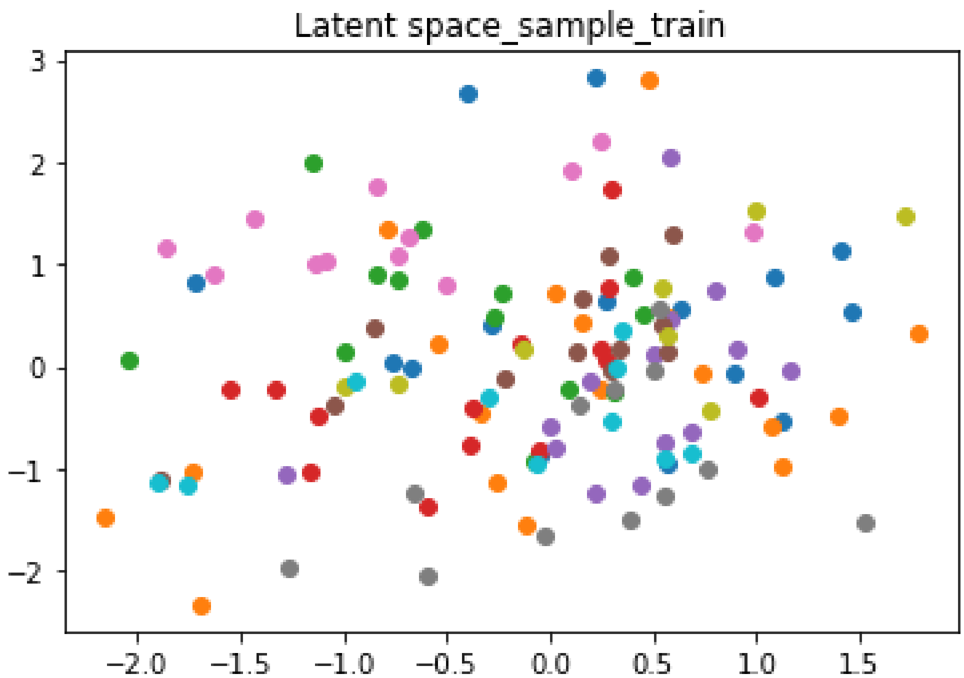
[27]:
```
model.eval()
sample_train_imgs, sample_train_labels = next(iter(train_loader))
print(sample_train_imgs.shape, sample_train_labels.shape)
sample_test_imgs, sample_test_labels = next(iter(test_loader))
print(sample_test_imgs.shape, sample_test_labels.shape)
sample_train_imgs, sample_test_imgs = torch.tensor(sample_train_imgs).float().
 ↪to(device), torch.tensor(sample_test_imgs).float().to(device)
sample_train_labels, sample_test_labels = torch.tensor(sample_train_labels).
 ↪to(device), torch.tensor(sample_test_labels).to(device)
```

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

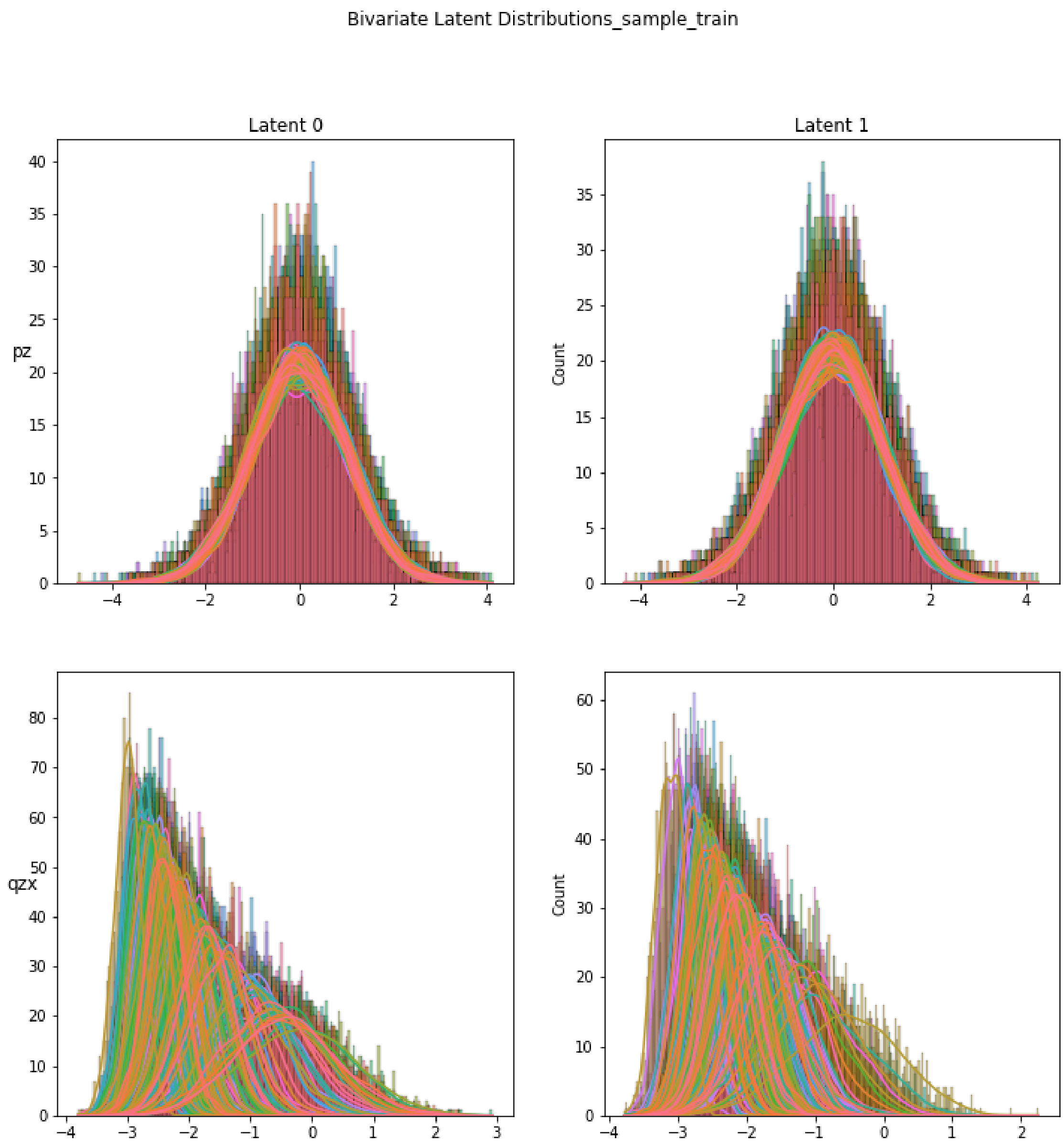
[28]:
```
sample_train_latents, sample_train_reconstructions, sample_train_latent_logvar,␣
 ↪sample_train_latent_logvar = model(sample_train_imgs, sample_train_labels)
sample_test_latents, sample_test_reconstructions, sample_test_latent_mean,␣
 ↪sample_test_latent_logvar = model(sample_test_imgs, sample_test_labels)
```

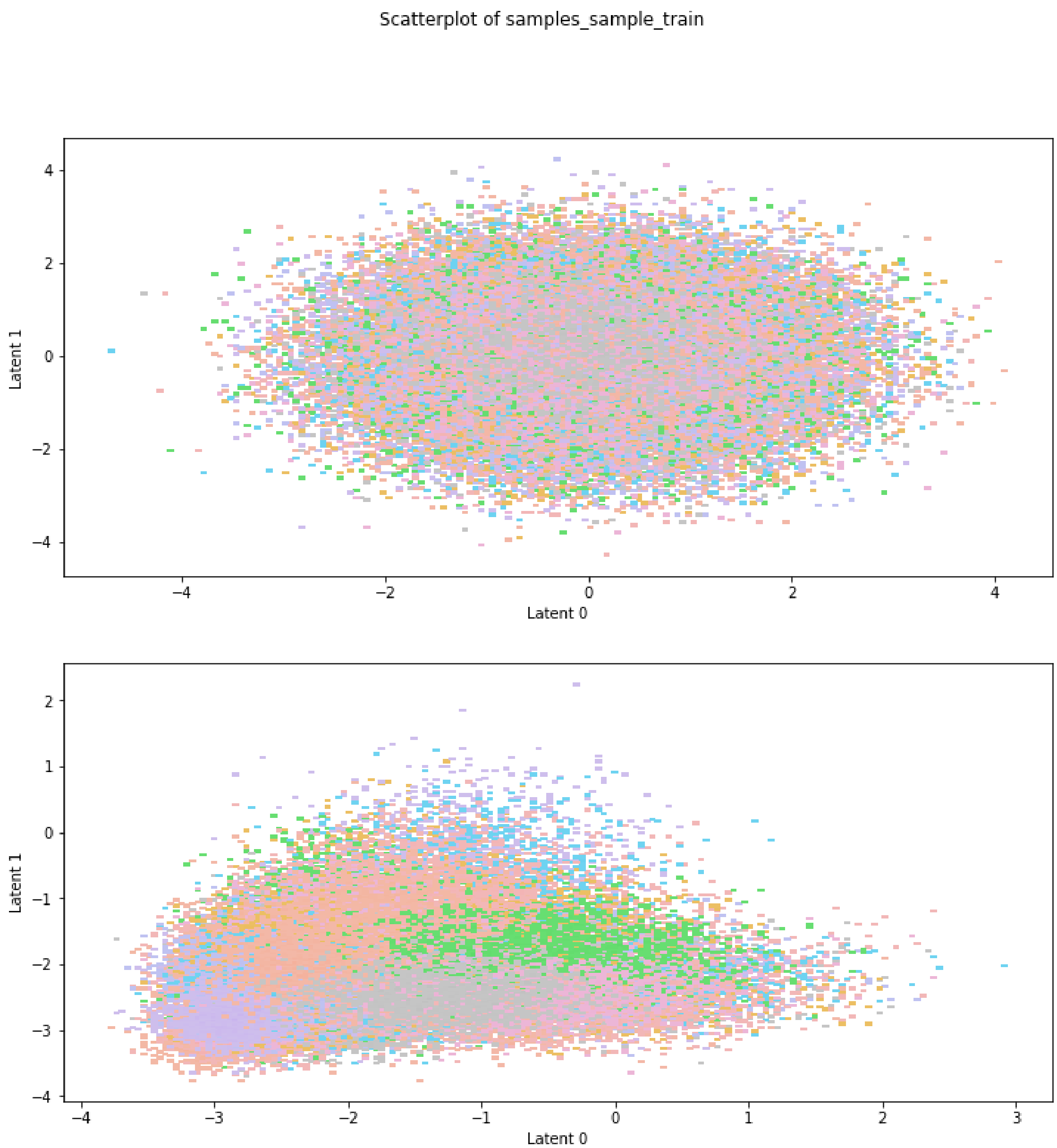
```
plot_latent(sample_train_labels, sample_train_latents, dtype="tensor",␣
 ↪suptitle_app="_sample_train")
plot_p_q(sample_train_latent_logvar, sample_train_latent_logvar,␣
 ↪N_samples=1000,suptitle_app="_sample_train")
plot_latent(sample_test_labels, sample_test_latents, dtype="tensor",␣
 ↪suptitle_app="_sample_test")
plot_p_q(sample_test_latent_mean, sample_test_latent_logvar, N_samples=1000,␣
 ↪suptitle_app="_sample_test")
```

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

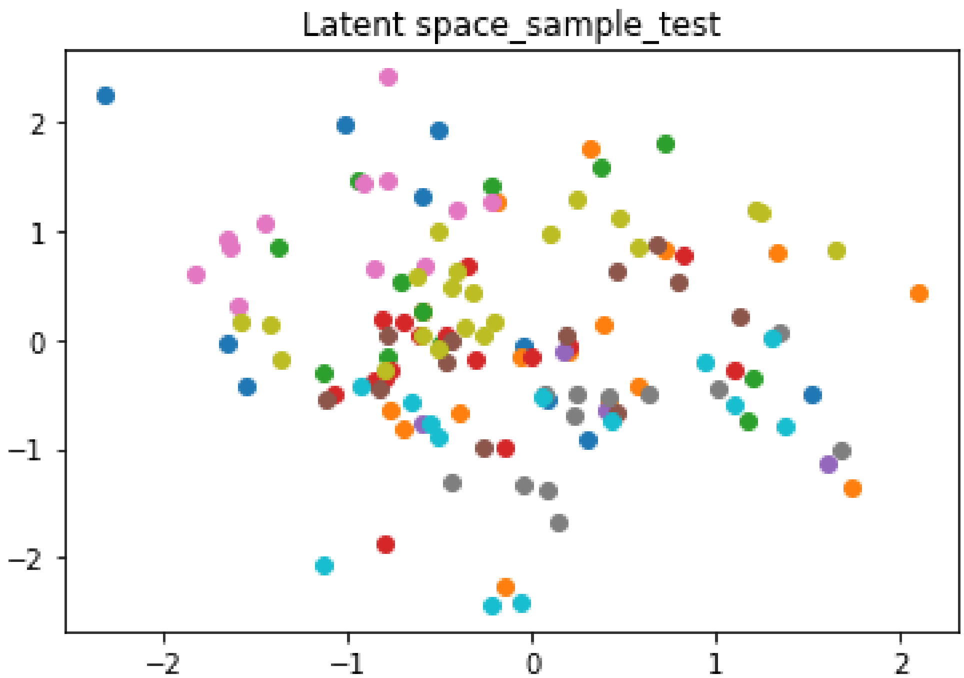



```
Plot bivariate latent distributions
pz batch_shape torch.Size([128, 2]), event_shape torch.Size([])
qzx batch_shape torch.Size([128, 2]), event_shape torch.Size([])
check p, q shape, pz (1000, 128, 2), qzx (1000, 128, 2)
```

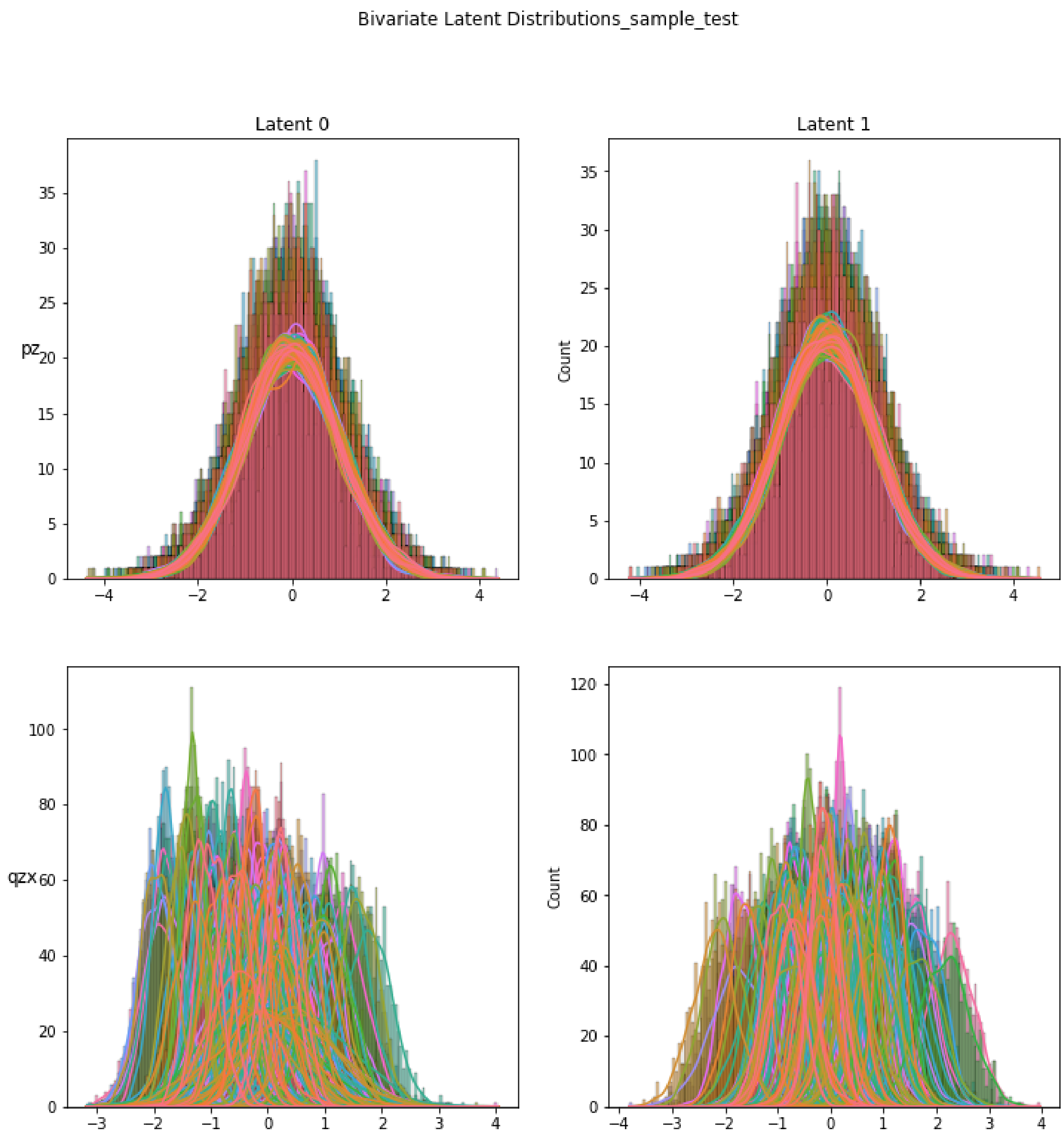

Bivariate Latent Distributions_sample_train
Latent 0
Latent 1
pz
qzx
Count
Count

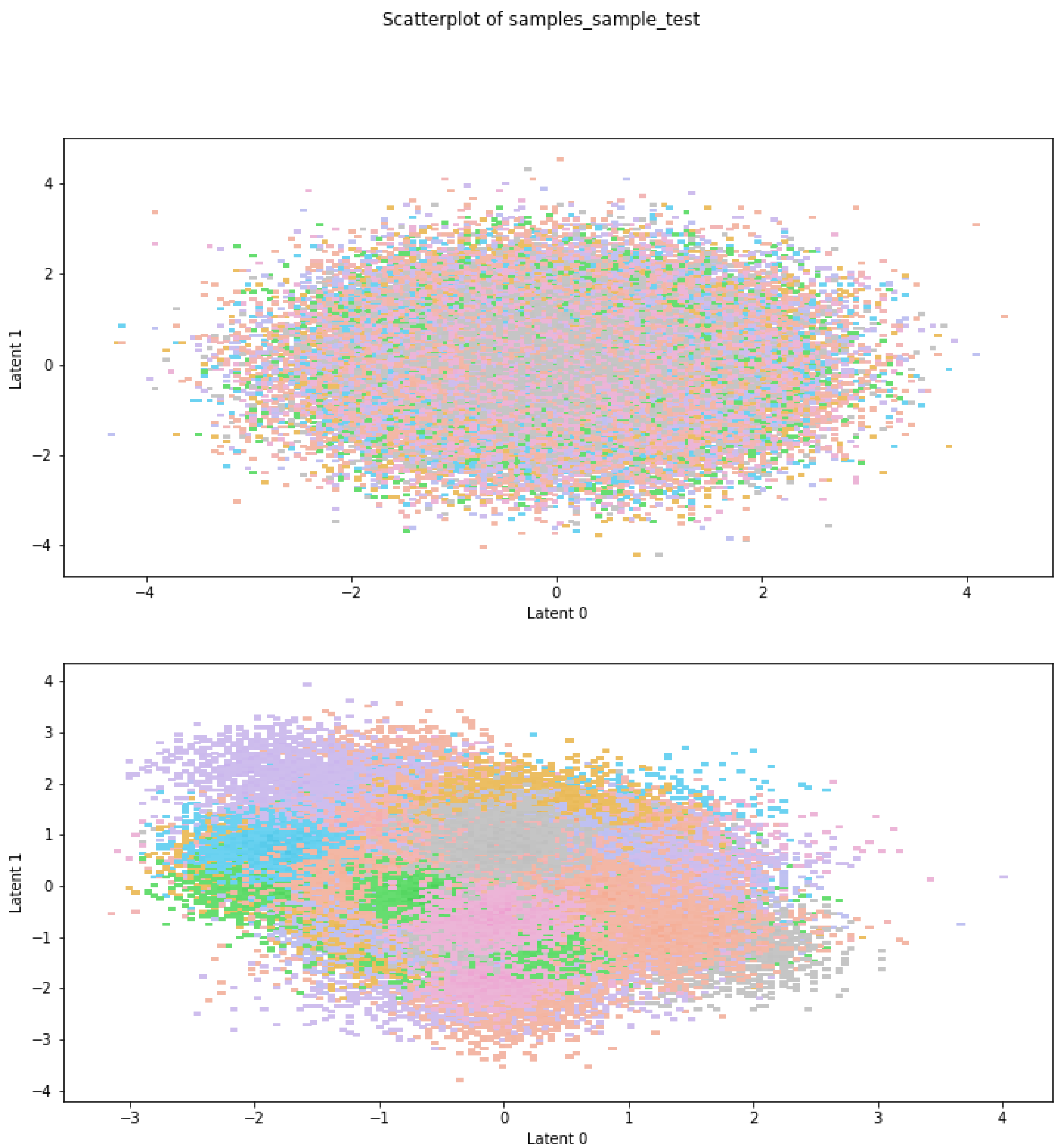



```
labels <class 'numpy.ndarray'> (128,)
latents <class 'numpy.ndarray'> (128, 2)
```




```
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 (1000, 128, 2), qzx (1000, 128, 2)
```


Bivariate Latent Distributions_sample_test
Latent 0
Latent 1
pz
Count
qzx
Count

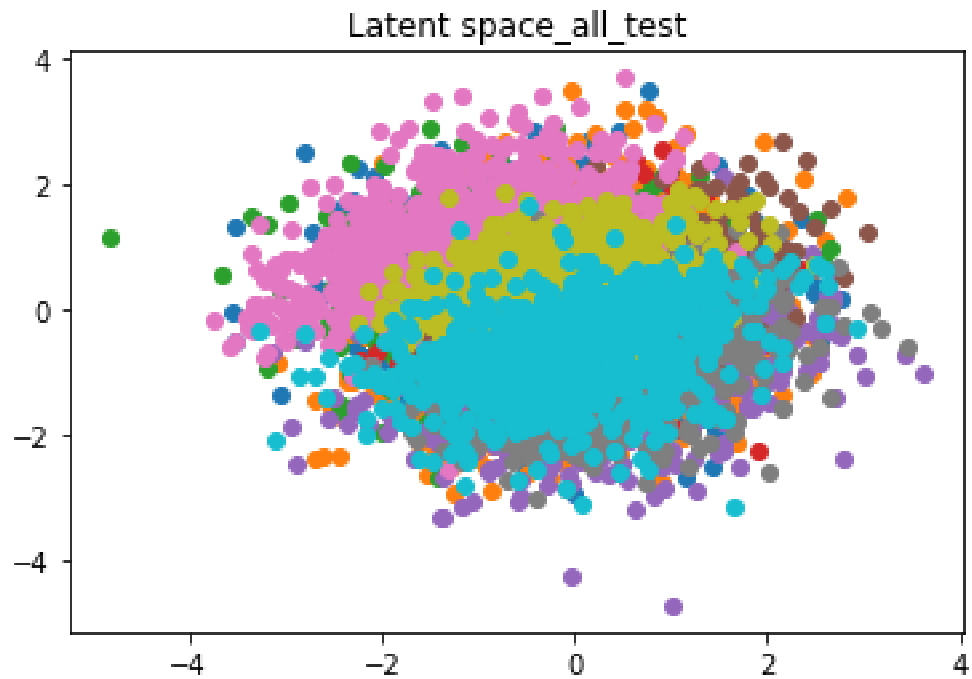


[29]:

```
# plot the whole test latent space
all_test_loader = torch.utils.data.DataLoader(test_dataset, batch_size=10000,␣
↪shuffle=True)
all_test_imgs, all_test_labels = next(iter(all_test_loader))
all_test_imgs, all_test_labels = torch.tensor(all_test_imgs).float().
↪to(device), torch.tensor(all_test_labels).to(device)
all_test_latents, all_test_reconstructions, all_test_latent_means,␣
↪all_test_latent_logvars = model(all_test_imgs, all_test_labels)
plot_latent(all_test_labels, all_test_latents, dtype="tensor",␣
↪suptitle_app="_all_test")
```

```
# plot_p_q(all_test_latent_means, all_test_latent_logvars, N_samples=1000,␣
↪suptitle_app="_sample_test") # takes forever
```

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



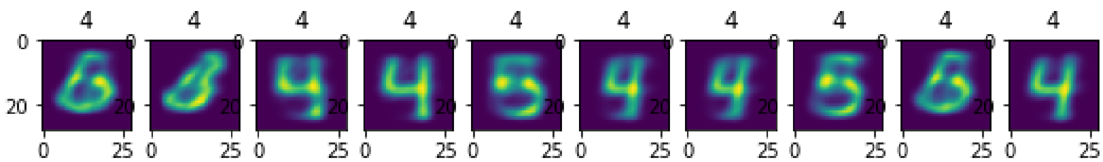
[30]:
```
all_test_latents = all_test_latents.cpu().detach().numpy()
all_test_labels = all_test_labels.cpu().detach().numpy()
```

3.4.4 Generate images conditioned on y

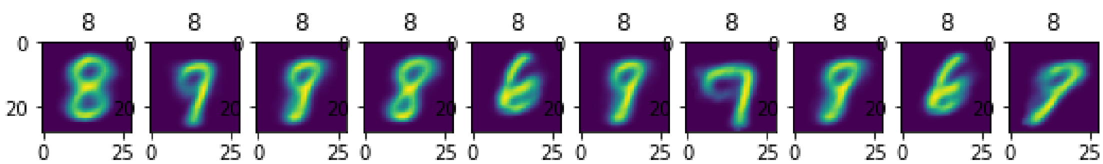
[31]:
```
def generate_data_cond_y(model, y, num_samples=10, latent_dim=2):
    if isinstance(y, int):
        y = np.repeat(y, num_samples)
    else:
        num_samples = len(y)

    y = torch.from_numpy(y).float().to(device)
    z = torch.randn(num_samples, latent_dim).to(device)
    assert z.shape[0]==y.shape[0], "inconsistent shape z {}, y {}".format(z.
↪shape, y.shape)
    recon_from_embeddings = model.decoder(z, y)
    y = y.cpu().detach().numpy(). astype(int)
```

```
    plt.figure(figsize=(num_samples,1))
    for i, recon in enumerate(recon_from_embeddings.cpu().detach().numpy()):
        plt.subplot(1, num_samples, i+1)
        plt.imshow(recon[0])
        plt.title("{}".format(y[i]))
#     plt.suptitle("Sampling for label {}".format(y))
```

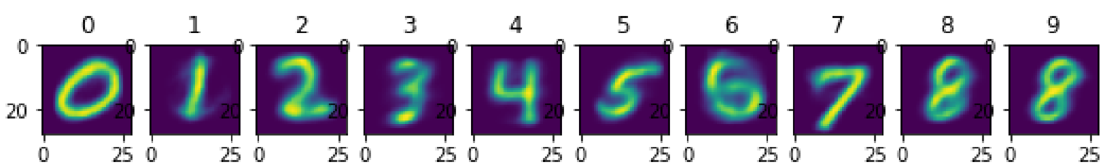
[32]:
```
y = 4
generate_data_cond_y(model, y, num_samples=10, latent_dim=2)
```



[33]:
```
y = 8
generate_data_cond_y(model, y, num_samples=10, latent_dim=2)
```



[34]:
```
y = np.arange(10)
generate_data_cond_y(model, y, latent_dim=2)
```



[ ]:
```
```