Problem 1.

$$
\begin{aligned}
D_{\mathrm{KL}}(q_T \parallel p) &= \int q_T(x) \log \frac{q_T(x)}{p(x)} dx \\
&= \int q(y) T(x|y) \log \frac{q_T(x)}{p(x)} dx dy \\
&\leq \int q(y) \log(\int \frac{T(x|y) q_T(x)}{p(x)} dx) dy \\
&= \int q(y) \log(\int \frac{T(y|x) q_T(x)}{p(y)} dx) dy \qquad \text{(detailed balance condition)} \\
&= \int q(y) \log(\frac{q(y) \int T(y|x) q_T(x) dx}{q(y) p(y)}) dy \\
&= D_{\mathrm{KL}}(q \parallel p) + \int q(y) \log(\frac{\int T(y|x) q_T(x) dx}{q(y)}) dy \\
&\leq D_{\mathrm{KL}}(q \parallel p) + \log(\int T(y|x) q_T(x) dx dy) \\
&\leq D_{\mathrm{KL}}(q \parallel p)
\end{aligned}
$$

Problem 2.

I. $\mathcal{L}_K \leq \log p(x)$

$$
\begin{aligned}
\mathcal{L}_K(q) &= E_{\theta_1, \ldots, \theta_K \sim q(\theta)} \log(\frac{1}{K} \sum_{i=1}^{K} \frac{p(x, \theta_i)}{q(\theta_i)}) \\
&\leq \log(\frac{1}{K} \sum_{i=1}^{K} \int \frac{p(x, \theta_i)}{q(\theta_i)} q(\theta_i) d\theta) \\
&= \log p(x)
\end{aligned}
$$

II. $\mathcal{L}_K \geq \mathcal{L}_m$ for $k \geq m$, (Burda et al., 2015)

Let I $\subset \{1, \ldots, k\}$ with |I| = m be a uniformly distributed subset of distinct indices from $\{1, \ldots, k\}$

$$
\begin{aligned}
\mathcal{L}_K(q) &= E_{\theta_1, \ldots, \theta_K \sim q(\theta)} \log(\frac{1}{K} \sum_{i=1}^{K} \frac{p(x, \theta_i)}{q(\theta_i)}) \\
&= E_{\theta_1, \ldots, \theta_K \sim q(\theta)} \log E_{I = \{i_1, \ldots, i_m\}} (\frac{1}{m} \sum_{j=1}^{m} \frac{p(x, \theta_{i_j})}{q(\theta_{i_j})}) \\
&\geq E_{\theta_1, \ldots, \theta_K \sim q(\theta)} E_{I = \{i_1, \ldots, i_m\}} \log(\frac{1}{m} \sum_{j=1}^{m} \frac{p(x, \theta_{i_j})}{q(\theta_{i_j})}) \\
&= E_{\theta_1, \ldots, \theta_m \sim q(\theta)} \log(\frac{1}{m} \sum_{i=1}^{m} \frac{p(x, \theta_i)}{q(\theta_i)}) \\
&= \mathcal{L}_m(q)
\end{aligned}
$$

Problem 3.

3. (1) Derive the ELBO and gradient estimator (using the reparameterization trick) for a general normalizing flow model with a standard normal base distribution

ELBO:

$$
\begin{aligned}
\mathcal{L} &= \mathbb{E}_{q_k(z_k)} \log \frac{p(x, z_k)}{q_k(z_k)} \\
&= \mathbb{E}_{q_0(z_0)} \log p(x, z_k) - \mathbb{E}_{q_0(z_0)} \log q_0(z_0) - \sum_{k=1}^{K} \mathbb{E}_{q_0(z_0)} \log \left| det(\frac{\partial f_k(z_{k-1})}{\partial z_{k-1}}) \right| \quad (reparameterization) \\
& z_0 \sim N(0, 1), \quad z_k = f_k \circ f_{k-1} \circ \ldots \circ f_1(z_0) = g(z_0)
\end{aligned}
$$

Gradient estimator:

1. ELBO estimator:

$$
\mathcal{L} = \frac{1}{N} \sum_{i=1}^{N} \log p(x, g(z_{0,i})) - \frac{1}{N} \sum_{i=1}^{N} \log q_0(z_{0,i}) - \sum_{k=1}^{K} \frac{1}{N} \sum_{i=1}^{N} \log \left| det(\frac{\partial f_k(z_{k-1,i})}{\partial z_{k-1}}) \right|
$$

2. Gradient estimator:

$$
\nabla \mathcal{L} = \frac{1}{N} \sum_{i=1}^{N} \nabla \log p(x, g(z_{0,i})) - \sum_{k=1}^{K} \frac{1}{N} \sum_{i=1}^{N} \nabla \log \left| det(\frac{\partial f_k(z_{k-1,i})}{\partial z_{k-1}}) \right|
$$

3. (2) Implement the following normalizing flows: planar flows, NICE and RealNVP.

In [44]:
```
import torch
import torch.nn as nn
from tqdm import tqdm
import numpy as np
from torch.nn import functional as F
import matplotlib.pyplot as plt
plt.rcParams['text.usetex'] = True
from numpy.random import uniform,exponential,chisquare,normal,randint, shuffle
torch.manual_seed(2022)
from torch.utils.data import Dataset
from torchvision import datasets
from torchvision.transforms import ToTensor
from torch.utils.data import DataLoader
from matplotlib.pyplot import imshow
from torchvision.utils import make_grid
```

In [120]:
```
data = np.load('banana_shape_data.npy')
```

In [121]:
```
data.shape
```

Out[121]: (100,)

planar flows

In [139]:
```
def log_joint_pdf(x, zk):
    sigma_y = torch.tensor(2)
    sigma_theta = torch.tensor(1)
    _t_ = torch.zeros(zk.shape[0]).to(device)
    for x_i in x:
        _t_ +=  - (x_i-zk[:,0]-zk[:,1]**2)**2/(2*sigma_y**2)
    return _t_ - (zk[:,0]**2+zk[:,1]**2)/(2*sigma_theta**2)

def ELBO(x, zk, log_jacobians):
    return (-log_jacobians - log_joint_pdf(x, zk)).mean()

class PlanarFlow(nn.Module):

    def __init__(self, data_dim=2):
        super().__init__()

        self.u = nn.Parameter(torch.rand(1, data_dim))
        self.w = nn.Parameter(torch.rand(1, data_dim))
        self.b = nn.Parameter(torch.rand(1))
        self.tanh = nn.Tanh()

    def forward(self, z):
        # transfrom
        activation = F.linear(z, self.w, self.b)
        x = z + self.u * self.tanh(activation)
        # log_det_jacobian
        psi = (1 - self.tanh(activation) ** 2) * self.w
        det_grad = 1 + torch.mm(psi, self.u.t())
        log_det_J = torch.log(det_grad + 1e-15)
        return x, log_det_J

class NormalizingFlowPlanar(nn.Module):

    def __init__(self, flow_length, data_dim=2):
        super().__init__()

        self.layers = nn.Sequential(
            *(PlanarFlow(data_dim) for _ in range(flow_length)))

    def forward(self, z):
        log_jacobians = 0
        for layer in self.layers:
            z, log_jacobian = layer(z)
            log_jacobians += log_jacobian
        return z, log_jacobians
```

In [142]:
```python
def train(flow, optimizer, nb_epochs, batch_size, data_dim, data):
    training_loss = []

    for epoch in tqdm(range(nb_epochs)):
        z0 = torch.randn(batch_size, data_dim).to(device)
        zk, log_jacobian = flow(z0)

        # backward prop
        optimizer.zero_grad()
        loss = ELBO(data, zk, log_jacobian)  # negative ELBO
        loss.backward()
        optimizer.step()

        training_loss.append(loss.item())

    return training_loss
```

In [143]:
```python
device = 'cpu'
flow_planar = NormalizingFlowPlanar(5).to(device)
optimizer = torch.optim.Adam(flow_planar.parameters(), lr=1e-2)
loss_planar = train(flow_planar, optimizer, 1000, 256, 2, data)
```

```
100%|██████████████████████████████████████████████████| 1000/1000 [00:10<00:00, 92.31it/s]
```

In [148]:
```python
def plot_ELBO(traces):
    loss = np.array(traces)
    elbo = -1*loss
    plt.plot(elbo, alpha=0.8)
    plt.xlabel("Epochs")
    plt.ylabel("ELBO")
    plt.show()
```

NICE

In [130]:
```python
class Coupling(nn.Module):
    def __init__(self, in_out_dim, mid_dim, hidden):
        super(Coupling, self).__init__()
        self.in_block = nn.Sequential(
            nn.Linear(in_out_dim//2, mid_dim),
            nn.ReLU())
        self.mid_block = nn.ModuleList([
            nn.Sequential(
                nn.Linear(mid_dim, mid_dim),
                nn.ReLU()) for _ in range(hidden - 1)])
        self.out_block = nn.Linear(mid_dim, in_out_dim//2)

    def forward(self, x, reverse=False):
        [B, W] = list(x.size())
        x = x.reshape((B, W//2, 2))
        off, on = x[:, :, 0], x[:, :, 1]
        off_ = self.in_block(off)
        for i in range(len(self.mid_block)):
            off_ = self.mid_block[i](off_)
        shift = self.out_block(off_)
        if reverse:
            on = on - shift
        else:
            on = on + shift
        x = torch.stack((on, off), dim=2)
        return x.reshape((B, W))

class Scaling(nn.Module):
    def __init__(self, dim):
        super(Scaling, self).__init__()
        self.scale = nn.Parameter(
            torch.zeros((1, dim)), requires_grad=True)

    def forward(self, x, reverse=False):
        log_det_J = torch.sum(self.scale)
        if reverse:
            x = x * torch.exp(-self.scale)
        else:
            x = x * torch.exp(self.scale)
        return x, log_det_J


class NormalizingFlowNICE(nn.Module):

    def __init__(self, coupling=3, in_out_dim=2, mid_dim=5, hidden=3):
        super(NormalizingFlowNICE, self).__init__()

        self.in_out_dim = in_out_dim

        self.coupling = nn.ModuleList([
            Coupling(in_out_dim=in_out_dim,
                     mid_dim=mid_dim,
                     hidden=hidden) \
            for i in range(coupling)])
        self.scaling = Scaling(in_out_dim)

    def forward(self, z):
        for i in range(len(self.coupling)):
            z = self.coupling[i](z)
        z, log_det_J = self.scaling(z)
        return z, log_det_J
```

In [131]:
```python
device = 'cpu'; data_dim = 2;
flow_nice = NormalizingFlowNICE().to(device)
optimizer = torch.optim.Adam(flow_nice.parameters(), lr=1e-2)
loss_nice = train(flow_nice, optimizer, 1000, 256, data_dim, data)
```

```
100%|██████████| 1000/1000 [00:11<00:00, 87.59it/s]
```

RealNVP

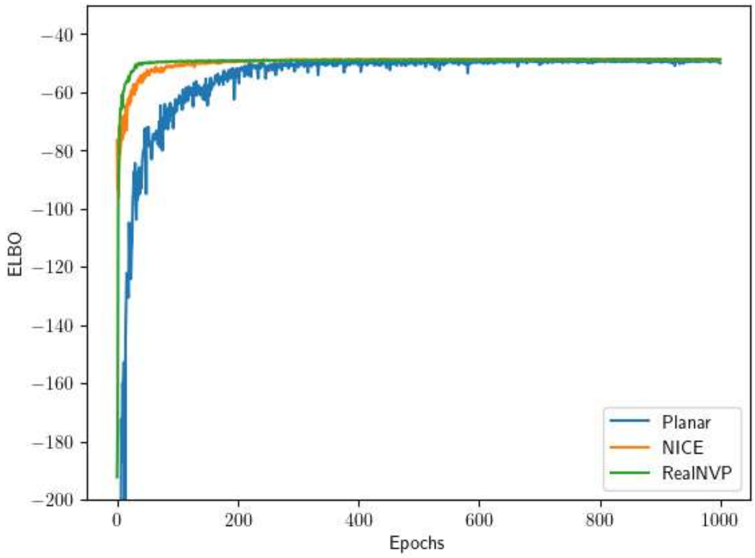
In [126]:
```python
class Scale(nn.Module):
    def __init__(self, in_out_dim, mid_dim, hidden):
        super(Scale, self).__init__()
        self.in_block = nn.Sequential(
            nn.Linear(in_out_dim//2, mid_dim),
            nn.ReLU())
        self.mid_block = nn.ModuleList([
            nn.Sequential(
                nn.Linear(mid_dim, mid_dim),
                nn.ReLU()) for _ in range(hidden - 1)])
        self.out_block = nn.Linear(mid_dim, in_out_dim//2)

    def forward(self, x, reverse=False):
        x = self.in_block(x)
        for i in range(len(self.mid_block)):
            off_ = self.mid_block[i](x)
        x = self.out_block(x)
        return x

class AffineCoupling(nn.Module):
    def __init__(self, in_out_dim=2, mid_dim=5, hidden=3):
        super(AffineCoupling, self).__init__()
        self.scale = Scale(in_out_dim=in_out_dim, mid_dim=mid_dim, hidden=hidden)
        self.translate = Scale(in_out_dim=in_out_dim, mid_dim=mid_dim, hidden=hidden)

    def forward(self, x):
        [B, W] = list(x.size())
        x = x.reshape((B, W//2, 2))
        off, on = x[:, :, 0], x[:, :, 1]
        # transform
        scale = self.scale(off)
        translate = self.translate(off)
        on = on*torch.exp(scale) + translate
        x = torch.stack((on, off), dim=2)
        # Jacobian
        log_det_J = scale.sum(-1)
        return x.reshape((B, W)), log_det_J

class RealNVP(nn.Module):

    def __init__(self, flow_length):
        super().__init__()

        self.layers = nn.Sequential(
            *(AffineCoupling() for _ in range(flow_length)))

    def forward(self, z):
        log_jacobians = 0
        for layer in self.layers:
            z, log_jacobian = layer(z)
            log_jacobians += log_jacobian
        return z, log_jacobians
```

In [127]:
```python
device = 'cpu'; data_dim = 2;
flow_realnvp = RealNVP(5).to(device)
optimizer = torch.optim.Adam(flow_realnvp.parameters(), lr=1e-2)
loss_realnvp = train(flow_realnvp, optimizer, 1000, 256, data_dim, data)
```

```
100%|██████████| 1000/1000 [00:12<00:00, 78.77it/s]
```

Show the lower bound as a function of the number of iterations:

In [154]:
```
plt.plot(-np.array(loss_planar), label='Planar')
plt.plot(-np.array(loss_nice), label='NICE')
plt.plot(-np.array(loss_realnvp), label='RealNVP')
plt.legend()
plt.xlabel("Epochs")
plt.ylabel("ELBO")
plt.ylim(-200, -30)
plt.show()
```



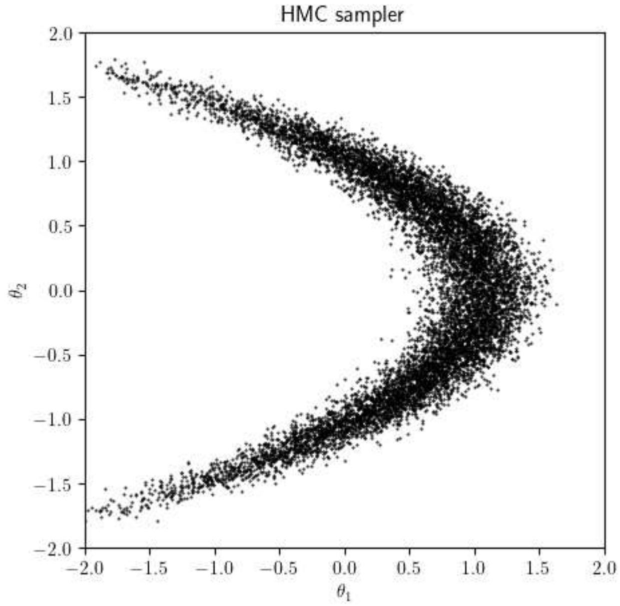
3. (3) Implement a Hamiltonian Monte Carlo sampler

In [159]:
```
def U(x, theta):
    """
    U(x) = -logP(x)
    """
    sigma_y = np.array(2)
    sigma_theta = np.array(1)
    return np.sum((x - theta[0]-theta[1]**2)**2)/(2*sigma_y**2) + (theta[0]**2+theta[1]**2)/(2*sigma_theta**2)

def dU(x, theta):
    sigma_y = np.array(2)
    sigma_theta = np.array(1)
    dtheta1 = -np.sum((x - theta[0]-theta[1]**2))/(sigma_y**2) + theta[0]/(sigma_theta**2)
    dtheta2 = -np.sum((x - theta[0]-theta[1]**2))*2*theta[1]/(sigma_y**2) + theta[1]/(sigma_theta**2)
    return np.array((dtheta1, dtheta2))


def HMC(data, initial, Lmax, step_size, fixed= True, epochs=1000):
    """
    Hamiltonian Monte Carlo
    :param initial: 初始点
    :param Lmax: 每轮次步数
    :param step_size: 步长
    :param epochs: 轮次
    :return: 样本
    """
    samples = [initial]
    for epoch in tqdm(range(epochs)):
        r = normal(0, 1, 2)  # 每轮epoch重新生成动量
        x = samples[-1]  # 上一次到达的位置
        # 先保存这次起点的位置
        x_prev = np.copy(x)
        r_prev = np.copy(r)
        # Simulate Hamiltonian dynamics
        if fixed:
            L = Lmax
        else:
            L = randint(1, Lmax+1)
        for step in range(L):
            # Leap-frog积分
            r = r - 0.5 * step_size * dU(data, x)  # 加上势函数的负梯度
            x = x + step_size * r  # 这里取的质量都是1
            r = r - 0.5 * step_size * dU(data, x)
        # flip the sign of the momentum
        r = -r
        # 计算接受概率
        ratio = np.exp(-(U(data, x) + 0.5 * r @ r) + (U(data, x_prev) + 0.5 * r_prev @ r_prev))
        accept = 1 if 1 < ratio else ratio
        u = uniform(0, 1)
        if u <= accept:
            samples.append(x)
        else:
            samples.append(x_prev)
    return np.array(samples)
```

In [160]:
```
initial = np.array([1.0, 0.5])
hmc_trace = HMC(data, initial, Lmax = 30, step_size=0.05, fixed=True,epochs=20000)
```

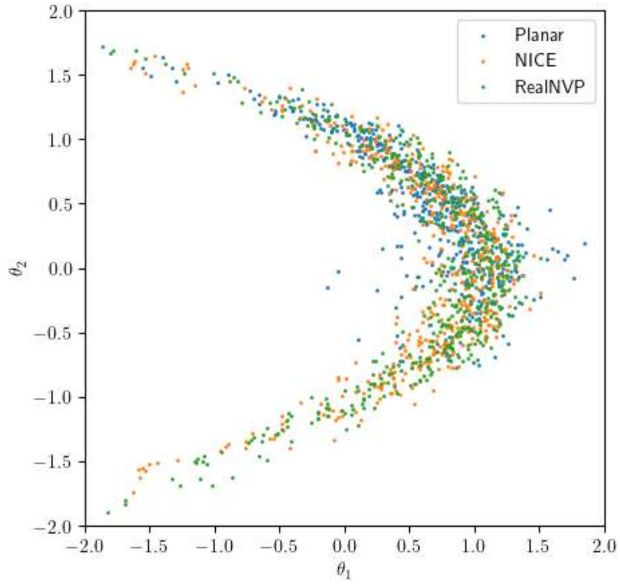
```
100%|██████████████████████████████████████████████████| 20000/20000 [00:14<00:00, 1341.81it/s]
```

In [161]:
```python
def scatter_2d(data):
    plt.figure(figsize=(5, 5))
    plt.scatter(data[10000:,0], data[10000:,1], marker='.', c = "black", s=1)
    # plt.legend()
    plt.xlabel(r"$ \theta_{1} $")
    plt.ylabel(r"$ \theta_{2} $")
    plt.title("HMC sampler")
    plt.ylim(-2, 2)
    plt.xlim(-2, 2)
    plt.show()
scatter_2d(hmc_trace)
```



3. (4) Show the scatter plots of these samples and compare to your HMC results. Report the KL divergence to the ground truth

In [162]:
```python
with torch.no_grad():
    z = torch.randn(500,2)
    zk_planar,_ = flow_planar(z.to(device))
    zk_nice,_ = flow_nice(z.to(device))
    zk_realnvp,_ = flow_realnvp(z.to(device))
plt.figure(figsize=(5, 5))
plt.scatter(zk_planar[:,0], zk_planar[:,1], label="Planar", s=1)
plt.scatter(zk_nice[:,0], zk_nice[:,1], label="NICE", s=1)
plt.scatter(zk_realnvp[:, 0], zk_realnvp[:, 1], label="RealNVP", s=1)
plt.legend()
plt.ylim(-2, 2)
plt.xlim(-2, 2)
plt.xlabel(r"$ \theta_{1} $")
plt.ylabel(r"$ \theta_{2} $")
plt.show()
```



In [156]:
```python
import ite
```

In [157]:
```
co = ite.cost.BDKL_KnnK()
```

In [165]:
```
with torch.no_grad():
    z = torch.randn(10000,2)
    planar_trace ,_ = flow_planar(z.to(device))
    nice_trace ,_ = flow_nice(z.to(device))
    realnvp_trace,_ = flow_realnvp(z.to(device))
```

In [167]:
```
kl_planar = co.estimation(planar_trace, hmc_trace[10000:])
kl_nice = co.estimation(nice_trace, hmc_trace[10000:])
kl_realnvp = co.estimation(realnvp_trace, hmc_trace[10000:])
print("KL divergence of Planar:\t%.3f"%kl_planar)
print("KL divergence of NICE:\t\t%.3f"%kl_nice)
print("KL divergence of RealNVP:\t%.3f"%kl_realnvp)
```

```
KL divergence of Planar:        0.507
KL divergence of NICE:          0.055
KL divergence of RealNVP:       0.075
```

NICE和RealNVP的KL divergence相对Planar明显更低，他们的抽样结果（上图）都比较好

Problem 4.

4. (1) Derive the evidence lower bound (ELBO) on the log likelihood of the model for N data points

$$
\begin{aligned}
\mathcal{L}(x;\theta,\phi) &= \sum_{i=1}^{N} \mathbb{E}_{q_{\phi,i}} \log \frac{p_\theta(x_i,z_i)}{q_{\phi,i}(z_i|x_i)} \\
&= \sum_{i=1}^{N} \mathbb{E}_{q_{\phi,i}} \log p_\theta(x_i|z_i) + \log p(z_i) - \log q_{\phi,i}(z_i|x_i) \\
&= \sum_{i=1}^{N} \mathbb{E}_{q_{\phi,i}} \log p(x_i|z_i;\theta) \text{ (reconstruction loss)} - KL(q_{\phi,i}(z_i|x_i)||p(z_i)) \\
&\text{where } \ KL(q_{\phi,i}(z_i|x_i) = \frac{1}{2}(1+\log(\sigma_i^2) - \mu_i^2 - \sigma_i^2) \text{ for gaussian prior}
\end{aligned}
$$

4. (2) Derive the gradient of the ELBO using the reparameterization trick. Briefly describe the advantages and disadvantages of VAE

1. Gradient with respect to θ :

$$
\begin{aligned}
\nabla_\theta \mathcal{L}(x;\theta,\phi) &= \nabla_\theta \sum_{i=1}^{N} \mathbb{E}_{q_{\phi,i}} \log \frac{p_\theta(x_i,z_i)}{q_{\phi,i}(z_i|x_i)} \\
&= \sum_{i=1}^{N} \mathbb{E}_{q_{\phi,i}} \nabla_\theta \log p_\theta(x_i,z_i) \\
&\approx \sum_{i=1}^{N} \frac{1}{K} \sum_{k=1}^{K} \nabla_\theta \log p_\theta(x_i,z_{i,k}) \qquad z_{i,k} \text{ are samples from } q_{\phi,i}(z)
\end{aligned}
$$

2. Gradient with respect to ϕ :

$$
\begin{aligned}
\nabla_\phi \mathcal{L}(x;\theta,\phi) &= \nabla_\phi \sum_{i=1}^{N} \mathbb{E}_{q_{\phi,i}} \log \frac{p_\theta(x_i,z_i)}{q_{\phi,i}(z_i|x_i)} \\
&= \sum_{i=1}^{N} \mathbb{E}_{q_\epsilon} \left(\nabla_\phi \log p_\theta(x_i, g_{\phi,i}(\epsilon)) - \nabla_\phi \log q_{\phi,i}(g_{\phi,i}(\epsilon))\ \right) \\
&= \sum_{i=1}^{N} \frac{1}{K} \sum_{k=1}^{K} \left(\nabla_\phi \log p_\theta(x_i, g_{\phi,i}(\epsilon_k)) - \nabla_\phi \log q_{\phi,i}(g_{\phi,i}(\epsilon_k))\ \right) \quad \epsilon_k \text{ are samples from } q_\epsilon(\epsilon_k)
\end{aligned}
$$

3. (reparameterization) transformation from ϵ to z:

$$
\begin{aligned}
z_i &= \mu + \sigma\epsilon, \quad \epsilon \sim \mathcal{N}(0,1) \\
\mu, \sigma &= f_\lambda(x_i) \quad f_\lambda \text{ is a neural network with parameter } \lambda
\end{aligned}
$$

4. advantages and disadvantages:

- VAE的优点在于其隐变量空间是连续的，方便生成新的样本（相对于普通Autoencoder而言）
- ELBO相对于GAN来讲可能更方便训练（收敛性）
- VAE的不足是对z采样重建过程中引入了采样噪声，重建的图形比较模糊

4. (3) Implement and train this VAE model for about 100 epochs.

In [60]:
```
class VAE(nn.Module):
    def __init__(self, input_dim = 28*28, enc_out_dim=512, latent_dim = 2):
        super(VAE, self).__init__()
        self.encoder = nn.Sequential(
            nn.Linear(input_dim, enc_out_dim),
            nn.ReLU()
        )

        self.decoder =  nn.Sequential(
            nn.Linear(latent_dim, enc_out_dim),
            nn.ReLU(),
            nn.Linear(enc_out_dim, input_dim)
        )
        self.fc_var = nn.Linear(enc_out_dim, latent_dim)
        self.log_scale = nn.Parameter(torch.Tensor([0.0]))

    def log_pxz(self, x_hat, logscale, x):
        scale = torch.exp(logscale)
        mean = x_hat
        dist = torch.distributions.Normal(mean, scale)
        log_pxz = dist.log_prob(x)
        return log_pxz.sum(dim=(1, 2, 3))

    def kl_divergence(self, z, mu, std):
        # p(z): normal prior
        p = torch.distributions.Normal(torch.zeros_like(mu), torch.ones_like(std))
        # p(z|x)
        q = torch.distributions.Normal(mu, std)
        log_qzx = q.log_prob(z)
        log_pz = p.log_prob(z)
        # sum of samples (apply mean to get KL)
        kl = (log_qzx - log_pz)
        kl = kl.sum(-1)
        return kl

    def forward(self, x):
        # encoder
        x_encoded = self.encoder(self.flatten(x))
        mu, log_var = self.fc_mu(x_encoded), self.fc_var(x_encoded)
        # sample z from p(z|x)
        std = torch.exp(log_var / 2)
        q = torch.distributions.Normal(mu, std)
        z = q.rsample()
        # decoder
        x_hat = self.decoder(z).reshape((-1, 1, 28, 28))
        # compute ELBO loss
        # reconstruction loss
        recon_loss = self.log_pxz(x_hat, self.log_scale, x)
        # kl divergence to prior
        kl = self.kl_divergence(z, mu, std)
        # elbo
        elbo = (kl - recon_loss)
        elbo = elbo.mean()
        return z, x_hat, elbo
```

In [16]:
```
training_data = datasets.MNIST(
    root=".",
    train=True,
    download=False,
    transform=ToTensor()
)
test_data = datasets.MNIST(
    root=".",
    train=False,
    download=False,
    transform=ToTensor()
)
```

In [77]:
```
train_dataloader = DataLoader(training_data, batch_size=128, shuffle=True)
test_dataloader = DataLoader(test_data, batch_size=128, shuffle=True)
```

In [75]:
```
def train(dataloader, model, optimizer, epochs = 100):
    size = len(dataloader.dataset)
    for t in range(epochs):
        print(f"Epoch {t+1}\n-------------------------------")
        for batch, (X, y) in enumerate(dataloader):
            X = X.to(device) # GPU
            _, X_hat, loss = model(X)
            # Backpropagation
            optimizer.zero_grad()
            loss.backward()
            optimizer.step()
            if batch % 100 == 0:
                loss, current = loss.item(), batch * len(X)
                print(f"loss: {loss:>7f}  [{current:>5d}/{size:>5d}]")
```

In [78]:
```
device = 'cuda'
model = VAE().to(device)
optimizer = torch.optim.Adam(model.parameters(), lr=1e-3)
train(train_dataloader, model, optimizer, epochs = 100)
```

```
loss: -176.876007  [51200/60000]
Epoch 95
-------------------------------
loss: -199.779724  [    0/60000]
loss: -188.246338  [12800/60000]
loss: -202.240067  [25600/60000]
loss: -189.457642  [38400/60000]
loss: -192.323059  [51200/60000]
Epoch 96
-------------------------------
loss: -197.067902  [    0/60000]
loss: -200.079620  [12800/60000]
loss: -201.143463  [25600/60000]
loss: -203.916885  [38400/60000]
loss: -170.642654  [51200/60000]
Epoch 97
-------------------------------
loss: -197.735779  [    0/60000]
loss: -174.289185  [12800/60000]
loss: -200.752289  [25600/60000]
```

4. (4) Visualize a random sample of 100 MNIST digits on 10 × 10 tile grid.

In [87]:
```
def img_sampler(model, num_preds = 16):
    rand_v = torch.rand((num_preds, 2))
    p = torch.distributions.Normal(torch.zeros_like(rand_v), torch.ones_like(rand_v))
    z = p.rsample().to(device)
    with torch.no_grad():
        pred = model.decoder(z).reshape((-1, 1, 28, 28))
    img = make_grid(pred, nrow=10).permute(1, 2, 0).cpu().numpy()
    plt.figure(figsize=(8, 8))
    imshow(img, cmap="gray");
```

“fake” digits

In [88]:
```
img_sampler(model, num_preds = 100)
```

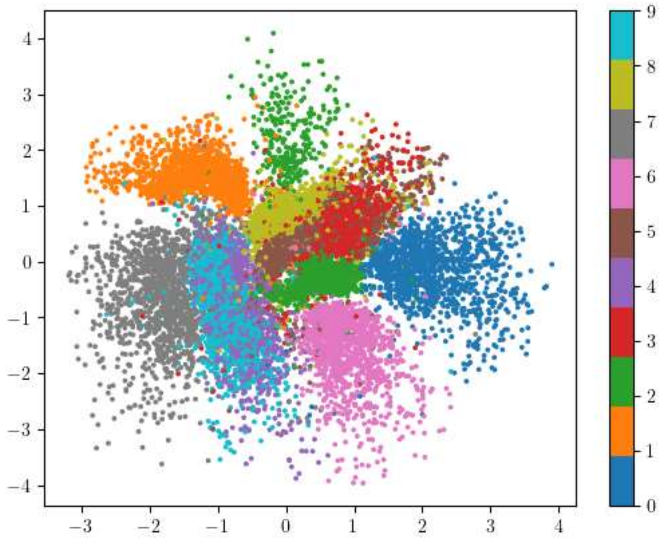
```
Clipping input data to the valid range for imshow with RGB data ([0..1] for floats or [0..255] for integers).
```

4. (5) Visualize the points in the latent space as a scatter plot, where colors of points should correspond to the labels of the digits

In [85]:
```
def plot_latent(model, data, num_batches=100):
    for i, (x, y) in enumerate(data):
        with torch.no_grad():
            x = x.to(device)
            z, _, _ = model(x)
            z = z.to('cpu').detach().numpy()
            plt.scatter(z[:, 0], z[:, 1], c=y, cmap='tab10', s=3)
            if i > num_batches:
                plt.colorbar()
                break
```

latent space

In [86]:
```
plot_latent(model, train_dataloader, num_batches=100)
```

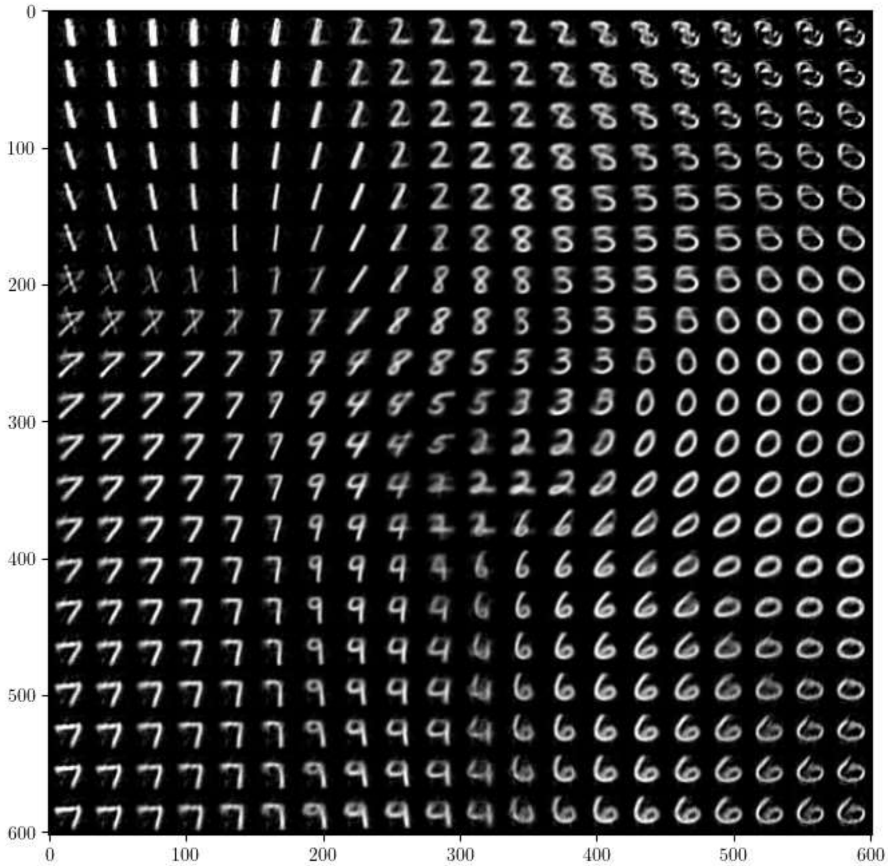


In [118]:
```
def plot_reconstructed(model):
    # 假设z1和z2的范围都是[-3, 3]
    x = torch.linspace(-3, 3, 20)
    y = torch.linspace(3, -3, 20)
    grid = torch.zeros((20*20, 2))
    # row by row
    for idy, i in enumerate(y):
        for idx, j in enumerate(x):
            grid[idy*20+idx, :] = torch.tensor((j, i))
    z = grid.to(device)
    with torch.no_grad():
        pred = model.decoder(z).reshape((-1, 1, 28, 28))
    img = make_grid(pred, nrow=20).permute(1, 2, 0).cpu().numpy()
    plt.figure(figsize=(8, 8))
    imshow(img, cmap="gray");
```

traversing latent space

In [119]:
```
plot_reconstructed(model)
```

```
Clipping input data to the valid range for imshow with RGB data ([0..1] for floats or [0..255] for integers).
```



In [ ]: