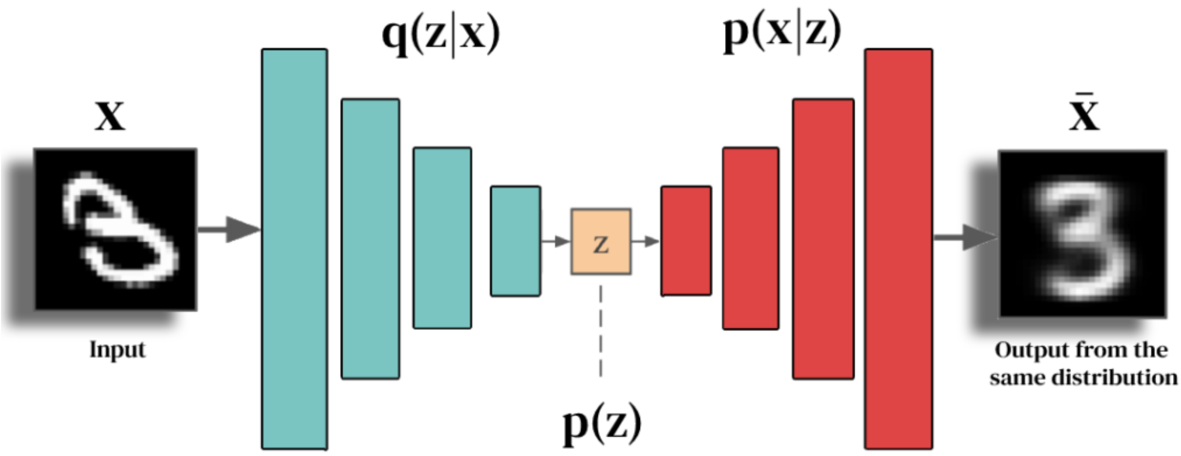
VAE for image generation

Consider VAE model from *Auto-Encoding Variational Bayes (2014, D.P. Kingma et. al.)*.

We will implement a VAE model using Torch and apply it to the MNIST dataset.



Generative model: We model each pixel value $\in \{0, 1\}$ as a sample drawn from a Bernoulli distribution. Through a decoder, the latent random variable z_n associated with an image n is mapped to the success parameters of the Bernoulli distributions associated with the pixels of that image. Our generative model is described as follows:

$z_n \sim N(0, I)$

$\theta_n = g(z_n)$

$x_n \sim Bern(\theta_n)$

where g is the decoder. We choose the prior on z_n to be the standard multivariate normal distribution, for computational convenience.

Inference model: We infer the posterior distribution of z_n via variational inference. The variational distribution $q(z_n|x_n)$ is chosen to be multivariate Gaussian with a diagonal covariance matrix. The mean and covariance of this distribution are obtained by applying an encoder to x_n.

$q(z_n|x_n) \sim q(\mu_n, \sigma_n^2)$

where $\mu_n, \sigma_n^2 = f(x_n)$ and f is the encoder.

Implementation: Let's start with importing Torch and other necessary libraries:

In [ ]:
```
import torch
import torch.nn as nn

import numpy as np

from tqdm import tqdm
from torchvision.utils import save_image, make_grid
```

Step1: Model Hyperparameters

In [ ]:
```
dataset_path = '~/datasets'

batch_size = 100

# Dimensions of the input, the hidden layer, and the latent space.
x_dim = 784
hidden_dim = 400
latent_dim = 200

# Learning rate
```

```
lr = 1e-3

# Number of epoch
epochs = 15  # can try something greater if you are not satisfied with the results
```

Step2: Load Dataset

In [ ]:
```
from torchvision.datasets import MNIST
import torchvision.transforms as transforms
from torch.utils.data import DataLoader

mnist_transform = transforms.Compose([
    transforms.ToTensor(),
])


train_dataset = MNIST(
    dataset_path, transform=mnist_transform, train=True, download=True)
test_dataset = MNIST(dataset_path, transform=mnist_transform,
                     train=False, download=True)

train_loader = DataLoader(dataset=train_dataset,
                          batch_size=batch_size, shuffle=True)
test_loader = DataLoader(dataset=test_dataset,
                         batch_size=batch_size, shuffle=False)
```

Step3: Define the model

In [ ]:
```
class Encoder(nn.Module):
    # encoder outputs the parameters of variational distribution "q"
    def __init__(self, input_dim, hidden_dim, latent_dim):
        super(Encoder, self).__init__()

        # FC stands for a fully connected layer
        self.FC_enc1 = nn.Linear(input_dim, hidden_dim)
        self.FC_enc2 = nn.Linear(hidden_dim, hidden_dim)
        self.FC_mean = nn.Linear(hidden_dim, latent_dim)
        self.FC_var = nn.Linear(hidden_dim, latent_dim)

        # will use this to add non-linearity to our model
        self.LeakyReLU = nn.LeakyReLU(0.2)

        self.training = True

    def forward(self, x):
        h_1 = self.LeakyReLU(self.FC_enc1(x))
        h_2 = self.LeakyReLU(self.FC_enc2(h_1))
        mean = self.FC_mean(h_2)  # mean
        log_var = self.FC_var(h_2)   # log of variance

        return mean, log_var
```

In [ ]:
```
class Decoder(nn.Module):
    # decoder generates the success parameter of each pixel
    def __init__(self, latent_dim, hidden_dim, output_dim):
        super(Decoder, self).__init__()
        self.FC_dec1 = nn.Linear(latent_dim, hidden_dim)
        self.FC_dec2 = nn.Linear(hidden_dim, hidden_dim)
        self.FC_output = nn.Linear(hidden_dim, output_dim)

        self.LeakyReLU = nn.LeakyReLU(0.2)  # again for non-linearity

    def forward(self, z):
        h_out_1 = self.LeakyReLU(self.FC_dec1(z))
        h_out_2 = self.LeakyReLU(self.FC_dec2(h_out_1))

        theta = torch.sigmoid(self.FC_output(h_out_2))
        return theta
```

Q3.1 (2 points) Below implement the reparameterization function.

In [ ]:
```
class Model(nn.Module):
    def __init__(self, Encoder, Decoder):
        super(Model, self).__init__()
        self.Encoder = Encoder
        self.Decoder = Decoder

    def reparameterization(self, mean, var):
        # insert your code here
        std = torch.sqrt(var + 1e-10)
        eps = torch.randn_like(std)
        z = mean + std * eps

        return z
```

```
    def forward(self, x):
        mean, log_var = self.Encoder(x)
        # takes exponential function (log var -> var)
        z = self.reparameterization(mean, torch.exp(log_var))

        theta = self.Decoder(z)

        return theta, mean, log_var
```

Step4: Model initialization

In [ ]:
```
encoder = Encoder(input_dim=x_dim, hidden_dim=hidden_dim,
                  latent_dim=latent_dim)


decoder = Decoder(latent_dim=latent_dim,
                  hidden_dim=hidden_dim, output_dim=x_dim)



model = Model(Encoder=encoder, Decoder=decoder)
```

Step5: Loss function and optimizer

Our objective function is ELBO: $E_{q(z|x)}\big[\log \frac{p(x,z)}{q(z|x)}\big]$

- **Q5.1 (1 point)** Show that ELBO can be rewritten as :

  $E_{q(z|x)}\big(\log p(x|z)\big) - D_{KL}\big(q(z|x)||p(z)\big)$

5.1 Your answer

$$\begin{aligned}
E_{q(z|x)}\big[\log \frac{p(x,z)}{q(z|x)}\big] &= E_{q(z|x)}\big[\log p(x,z) - \log q(z|x)\big] \\
&= E_{q(z|x)}\big[\log p(x|z) + \log p(z) - \log q(z|x)\big] \\
&= E_{q(z|x)}\big[\log p(x|z)\big] + E_{q(z|x)}\big[\log p(z)\big] - E_{q(z|x)}\big[\log q(z|x)\big] \\
&= E_{q(z|x)}\big[\log p(x|z)\big] - E_{q(z|x)}\big[\log \frac{q(z|x)}{p(z)}\big] \\
&= E_{q(z|x)}\big[\log p(x|z)\big] - D_{KL}\big(q(z|x)||p(z)\big)
\end{aligned}$$

Consider the first term: $E_{q(z|x)}\big(\log p(x|z)\big)$

$E\_q(z|x)\big(\log p(x|z)\big) = \int q(z|x) \log p(x|z) dz$

We can approximate this integral by Monte Carlo integration as following:

$\approx \frac{1}{L}\sum_{l=1}^{L} \log p(x|z_l)$, where $z_l \sim q(z|x)$.

Now we can compute this term using the analytic expression for $p(x|z)$. (Remember we model each pixel as a sample drawn from a Bernoulli distribution).

Consider the second term: $-D_{KL}\big(q(z|x)||p(z)\big)$

- **Q5.2 (2 points)** Kullback–Leibler divergence can be computed using the closed-form analytic expression when both the variational and the prior distributions are Gaussian. Write down this KL divergence in terms of the parameters of the prior and the variational distributions. Your solution should consider a generic case where the latent space is K-dimensional.

5.2 Your answer

$$
\begin{aligned}
D_{KL}\left(q(z|x)||p(z)\right) &= \int q(z|x)\log\frac{q(z|x)}{p(z)}\,dz \\
&= \int q(z|x)\log\frac{\prod_{i=1}^{K}\left(2\pi\sigma_i^2\right)^{-\frac{1}{2}}\exp\left(-\frac{(z_i-\mu_i)^2}{2\sigma_i^2}\right)}{\prod_{i=1}^{K}\left(2\pi\right)^{-\frac{1}{2}}\exp\left(-\frac{z_i^2}{2}\right)}\,dz \\
&= \int q(z|x)\left(\sum_{i=1}^{K}-\log(\sigma_i)-\frac{(z_i-\mu_i)^2}{2\sigma_i^2}+\frac{z_i^2}{2}\right)dz \\
&= \mathbb{E}_{q(z|x)}\left[\sum_{i=1}^{K}-\log(\sigma_i)-\frac{(z_i-\mu_i)^2}{2\sigma_i^2}+\frac{z_i^2}{2}\right] \\
&= \sum_{i=1}^{K}-\log(\sigma_i)-\frac{\mathbb{E}_{q(z|x)}\left[(z_i-\mu_i)^2\right]}{2\sigma_i^2}+\frac{\mathbb{E}_{q(z|x)}\left[z_i^2\right]}{2} \\
&= \sum_{i=1}^{K}-\log(\sigma_i)-\frac{\sigma_i^2}{2\sigma_i^2}+\frac{\mathbb{E}_{q(z|x)}[z_i^2]}{2} \\
&= \sum_{i=1}^{K}-\log(\sigma_i)-\frac{1}{2}+\frac{\sigma_i^2+\mu_i^2}{2} \\
D_{KL}\left(q(z|x)||p(z)\right) &= \frac{1}{2}\sum_{i=1}^{K}\left(\sigma_i^2+\mu_i^2-\log(\sigma_i^2)-1\right)
\end{aligned}
$$

Q5.3 (5 points) Now use your findings to implement the loss function, which is the negative of ELBO:

In [ ]:
```
from torch.optim import Adam


def loss_function(x, theta, mean, log_var):  # should return the loss function (- ELBO)
    # insert your code here
    # expected log-likelihood
    recon_loss = -torch.sum(x * torch.log(theta + 1e-10) +
                            (1 - x) * torch.log(1 - theta + 1e-10))

    # KL Divergence
    kl_div = -0.5 * torch.sum(1 + log_var - mean.pow(2) - log_var.exp())

    loss = recon_loss + kl_div

    return loss


# optimizer
optimizer = Adam(model.parameters(), lr=lr)
```

Step6: Train the model

In [ ]:
```
print("Start training VAE...")
model.train()

for epoch in range(epochs):
    overall_loss = 0
    for batch_idx, (x, _) in enumerate(train_loader):
        x = x.view(batch_size, x_dim)
        x = torch.round(x)

        optimizer.zero_grad()

        theta, mean, log_var = model(x)
        loss = loss_function(x, theta, mean, log_var)

        overall_loss += loss.item()

        loss.backward()
        optimizer.step()

    print("\tEpoch", epoch + 1, "complete!", "\tAverage Loss: ",
          overall_loss / (batch_idx*batch_size))

print("Finish!!")
```

```
Start training VAE...
	Epoch 1 complete! 	Average Loss:  170.46923104262314
	Epoch 2 complete! 	Average Loss:  119.11499233748957
	Epoch 3 complete! 	Average Loss:  104.68442185543614
	Epoch 4 complete! 	Average Loss:  98.1438308639399
	Epoch 5 complete! 	Average Loss:  94.27063854797058
	Epoch 6 complete! 	Average Loss:  91.71576331646494
	Epoch 7 complete! 	Average Loss:  90.0293065183509
	Epoch 8 complete! 	Average Loss:  88.59584846815004
	Epoch 9 complete! 	Average Loss:  87.54152457057336
	Epoch 10 complete! 	Average Loss:  86.68927987889973
	Epoch 11 complete! 	Average Loss:  85.85783046614148
	Epoch 12 complete! 	Average Loss:  85.21846442475741
	Epoch 13 complete! 	Average Loss:  84.57121777669815
	Epoch 14 complete! 	Average Loss:  84.07572356922996
	Epoch 15 complete! 	Average Loss:  83.5210108644616
Finish!!
```

Step7: Generate images from test dataset

With our model trained, now we can start generating images.

First, we will generate images from the latent representations of test data.

Basically, we will sample z from $q(z|x)$ and give it to the generative model (i.e., decoder) $p(x|z)$. The output of the decoder will be displayed as the generated image.

Q7.1 (2 points) Write a code to get the reconstructions of test data, and then display them using the show_image function

In [ ]:
```python
model.eval()
# below we get decoder outputs for test data
with torch.no_grad():
    for batch_idx, (x, _) in enumerate(tqdm(test_loader)):
        x = x.view(batch_size, x_dim)
        # insert your code below to generate theta from x

        # Pass the test images through the encoder and decoder
        mean, log_var = model.Encoder(x)
        # reparameterize to get latent variable
        z = model.reparameterization(mean, torch.exp(log_var))
        # decode the latent variable to get reconstructed image
        theta = model.Decoder(z)
```

```
100%|██████████████████████████████████████████████████| 100/100 [00:00<00:00, 111.61it/s]
```

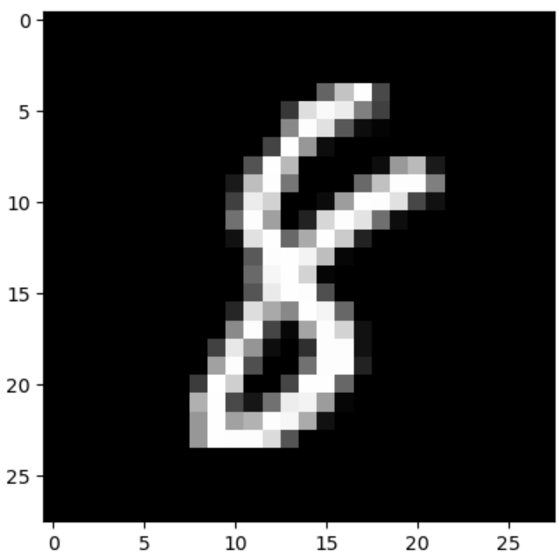
A helper function to display images:

In [ ]:
```python
import matplotlib.pyplot as plt


def show_image(theta, idx):
    x_hat = theta.view(batch_size, 28, 28)
    # x_hat = Bernoulli(x_hat).sample() # sample pixel values (you can also try this, and observe how the generated images l
    fig = plt.figure()
    plt.imshow(x_hat[idx].cpu().numpy(), cmap='gray')
```

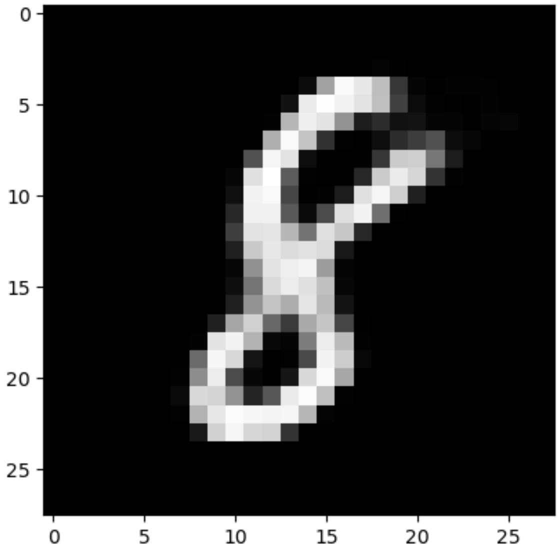
First display an image from the test dataset,

In [ ]:
```python
show_image(x, idx=0)  # try different indices as well
```



Now display its reconstruction and compare:

In [ ]:
```
show_image(theta, idx=0)
```



Step8: Generate images from noise

In the previous step, we sampled latent vector z from $q(z|x)$. However, we know that the KL term in our loss function enforced $q(z|x)$ to be close to $N(0, I)$. Therefore, we can sample z directly from noise $N(0, I)$, and pass it to the decoder $p(x|z)$.

Q8.1 (3 points) Create images from noise and display.

In [ ]:
```
with torch.no_grad():
    # insert your code here to create images from noise (it is enough to create theta value for each pixel)
    #
    #
    # generated_images = ....  # should be a matrix ( batch_size-by-x_dim )
    generated_images = torch.round(
        model.Decoder(torch.randn(batch_size, latent_dim)))
```

Display a couple of generated images:

In [ ]:
```
show_image(generated_images, idx=0)
```