Autoencoder
and
Variational Autoencoder

Physics 361 Machine Learning in Physics

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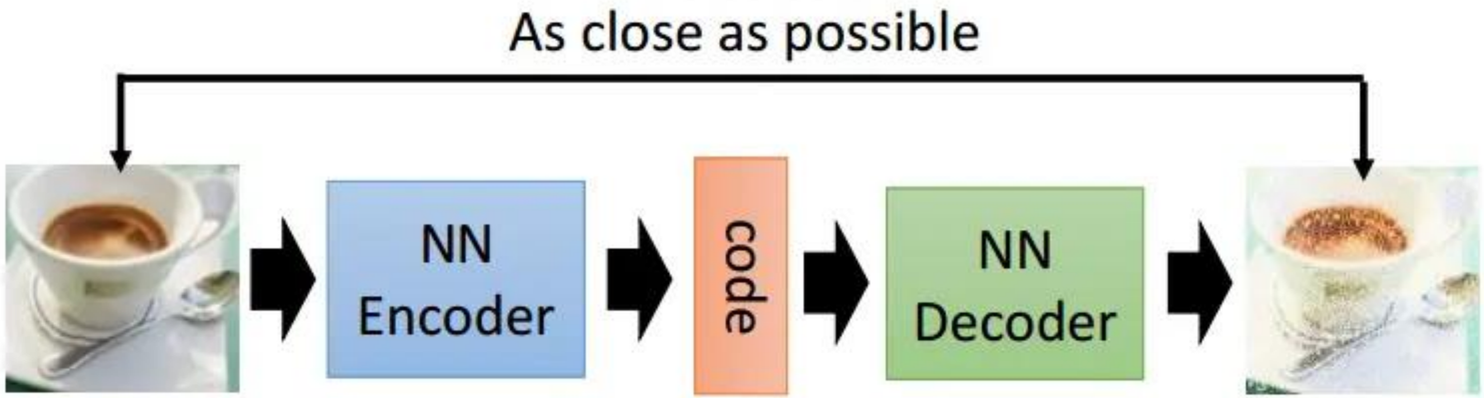
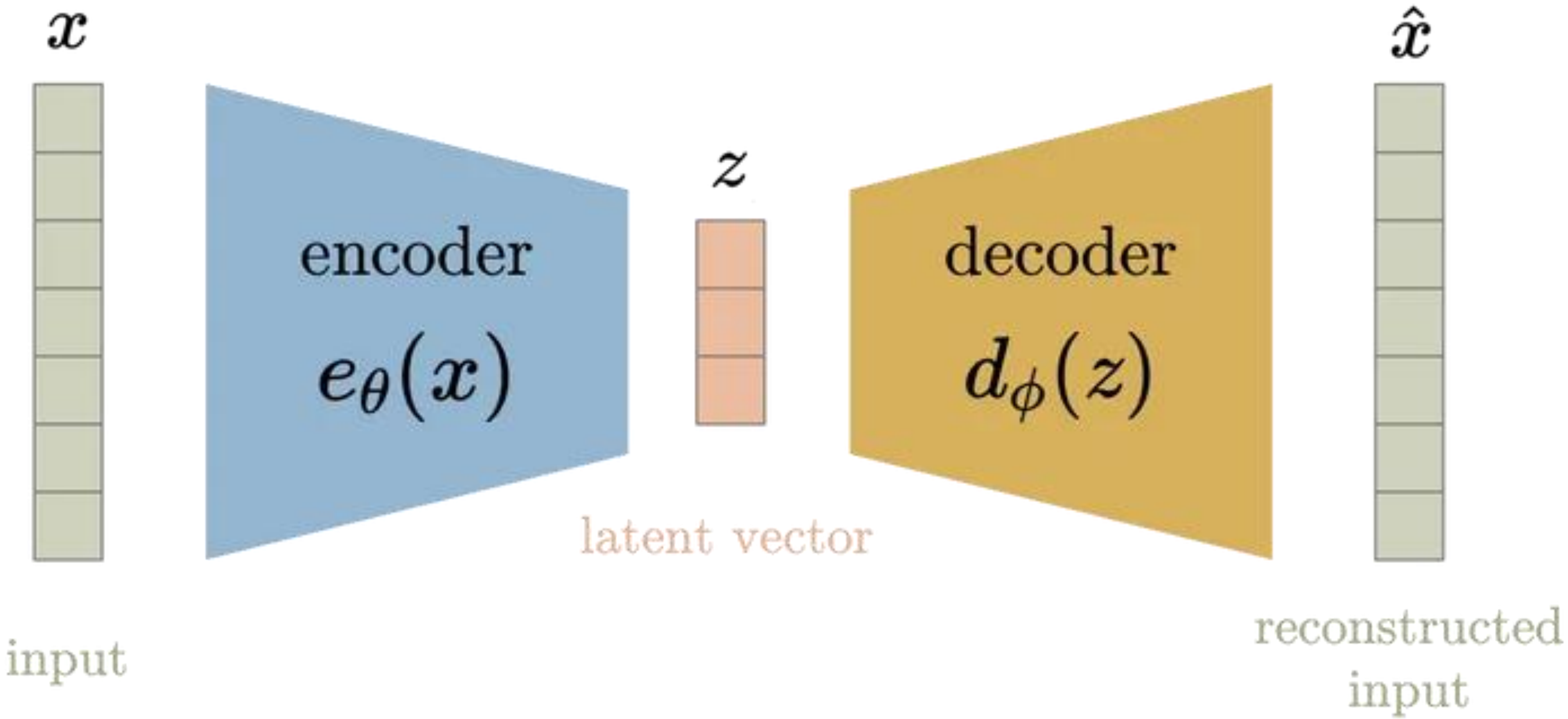
A quick look at the autoencoder



A quick look at the autoencoder



$$loss = \|x - \hat{x}\|_2^2$$

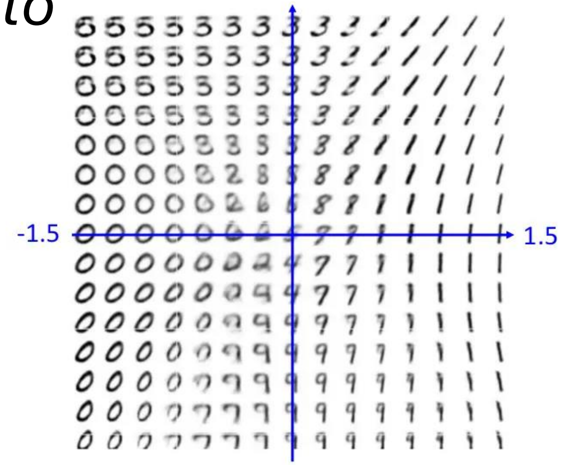
Why autoencoder (AE)

- Compression / dimensionality reduction
  - Curse of dimensionality
    - Exponential increase in required # of samples / peaking in predictive power
    - Loss of meaning for the distance function
  - Nonlinear analogue of PCA

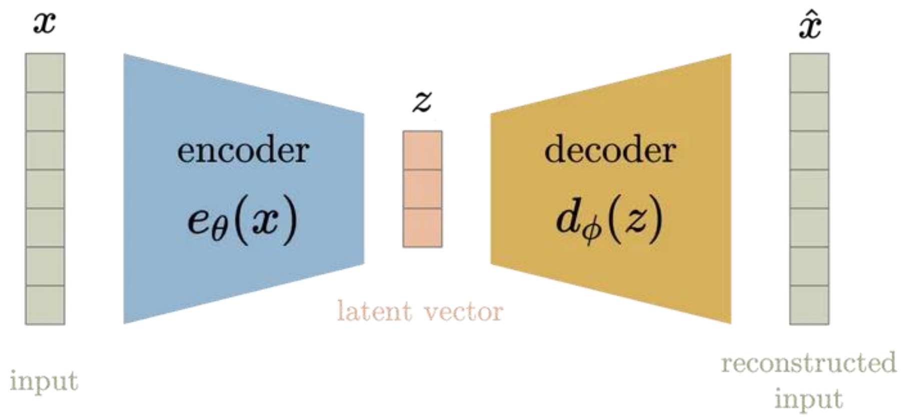
$$\frac{V_{\text{hypersphere}}}{V_{\text{hypercube}}} = \frac{\pi^{d/2}}{d2^{d-1}\Gamma(d/2)} \to 0$$

- Applications
  - Layer-wise (pre)training for deep networks *(depreciated due to batch normalization & ResNet)*
  - Training data preprocessing (compression, denoising)
  - Anomaly detection
  - **As a generative model (esp. variational autoencoder)**

latent space



AE – architectures



- Dimension of the latent space
  - Undercomplete & overcomplete autoencoders

- The encoder & decoder are just compression & decompression functions to be approximated by NNs

- Architecture depends on how data is represented
  - A vector: multilayer perceptron
  - A field: convolutional neural network
  - A graph: graph neural network

AE – implementations

MLP

```
class autoencoder(nn.Module):
    def __init__(self):
        super(autoencoder, self).__init__()
        self.encoder = nn.Sequential(
            nn.Linear(28 * 28, 128),
            nn.ReLU(True),
            nn.Linear(128, 64),
            nn.ReLU(True), nn.Linear(64, 12), nn.ReLU(True), nn.Linear(12, 3))
        self.decoder = nn.Sequential(
            nn.Linear(3, 12),
            nn.ReLU(True),
            nn.Linear(12, 64),
            nn.ReLU(True),
            nn.Linear(64, 128),
            nn.ReLU(True), nn.Linear(128, 28 * 28), nn.Tanh())

    def forward(self, x):
        x = self.encoder(x)
        x = self.decoder(x)
        return x
```

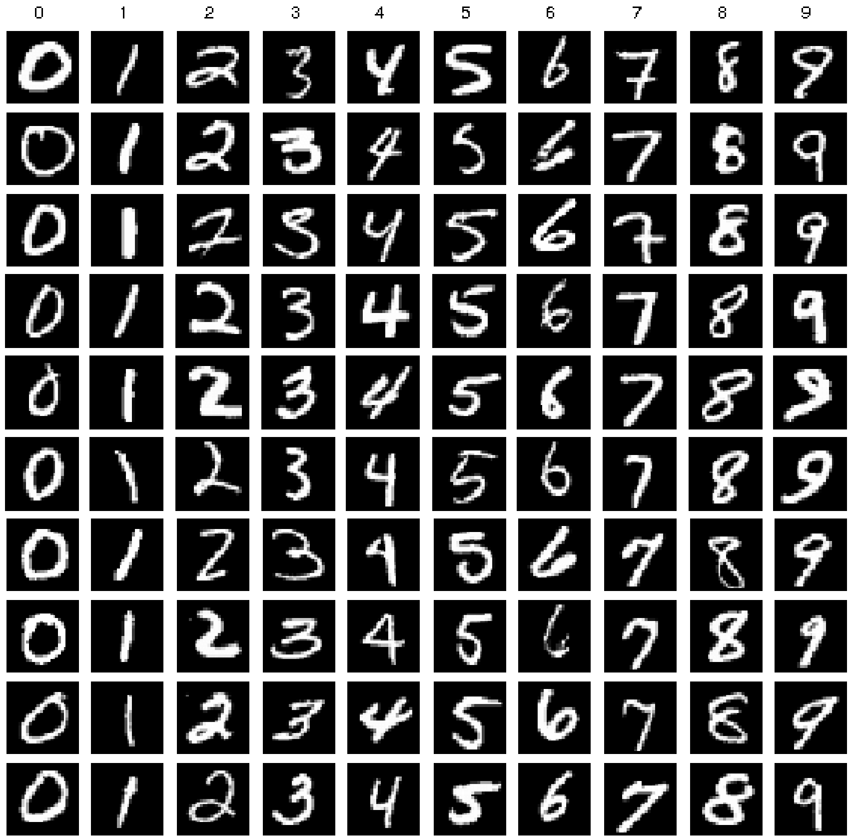
CNN

```
class autoencoder(nn.Module):
    def __init__(self):
        super(autoencoder, self).__init__()
        self.encoder = nn.Sequential(
            nn.Conv2d(1, 16, 3, stride=3, padding=1),  # b, 16, 10, 10
            nn.ReLU(True),
            nn.MaxPool2d(2, stride=2),  # b, 16, 5, 5
            nn.Conv2d(16, 8, 3, stride=2, padding=1),  # b, 8, 3, 3
            nn.ReLU(True),
            nn.MaxPool2d(2, stride=1)  # b, 8, 2, 2
        )
        self.decoder = nn.Sequential(
            nn.ConvTranspose2d(8, 16, 3, stride=2),  # b, 16, 5, 5
            nn.ReLU(True),
            nn.ConvTranspose2d(16, 8, 5, stride=3, padding=1),  # b, 8, 15, 15
            nn.ReLU(True),
            nn.ConvTranspose2d(8, 1, 2, stride=2, padding=1),  # b, 1, 28, 28
            nn.Tanh()
        )

    def forward(self, x):
        x = self.encoder(x)
        x = self.decoder(x)
        return x
```

AE – implementations

```
model = autoencoder().cuda()
criterion = nn.MSELoss()
optimizer = torch.optim.Adam(model.parameters(), lr=learning_rate,
                             weight_decay=1e-5)

for epoch in range(num_epochs):
    total_loss = 0
    for data in dataloader:
        img, _ = data
        img = Variable(img).cuda()
        # ===================forward=====================
        output = model(img)
        loss = criterion(output, img)
        # ===================backward====================
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
        total_loss += loss.data
```

AE – reconstruction examples



MNIST dataset

AE

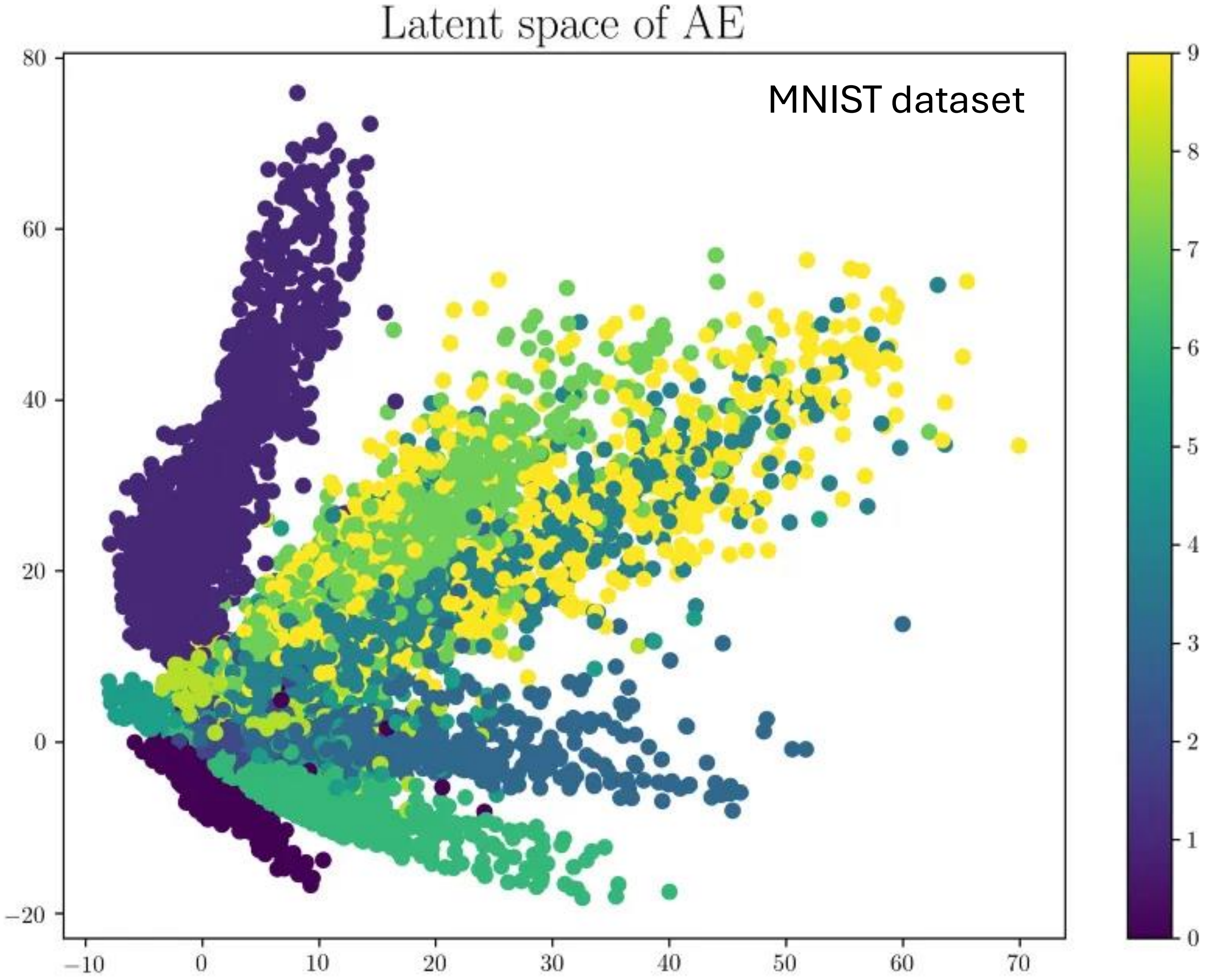
MLP

blurry?

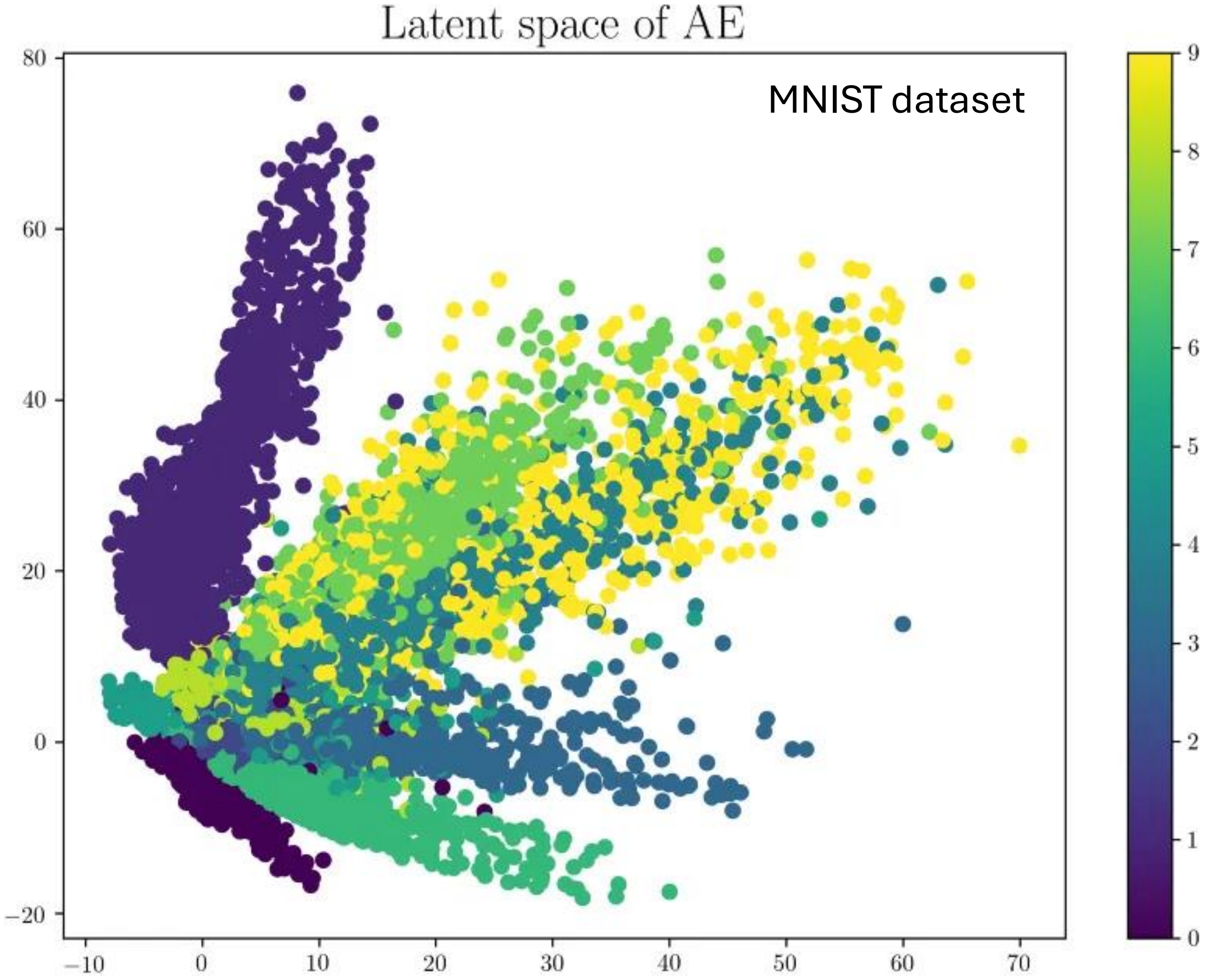
CNN

more details?

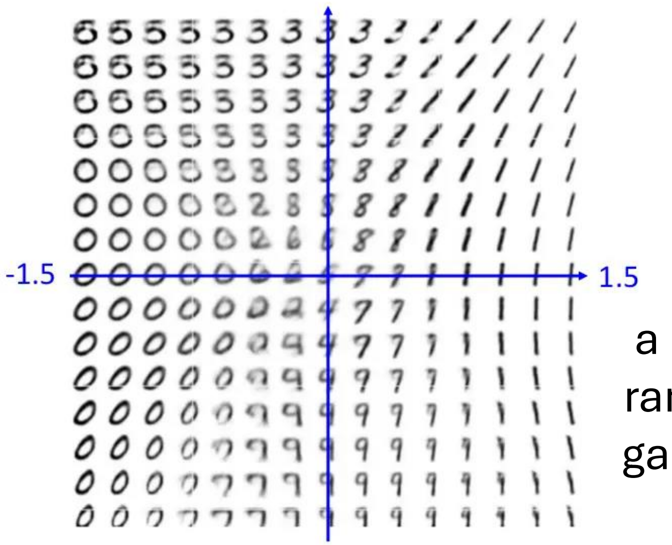
AE – latent space



AE – latent space



- **Clustering:** same digits are close to each other in the latent space
- **Empty space:** regions outside of clusters cannot be used for data generation – **the latent space is not regularized**



a lot of random garbage

AE – regularizations

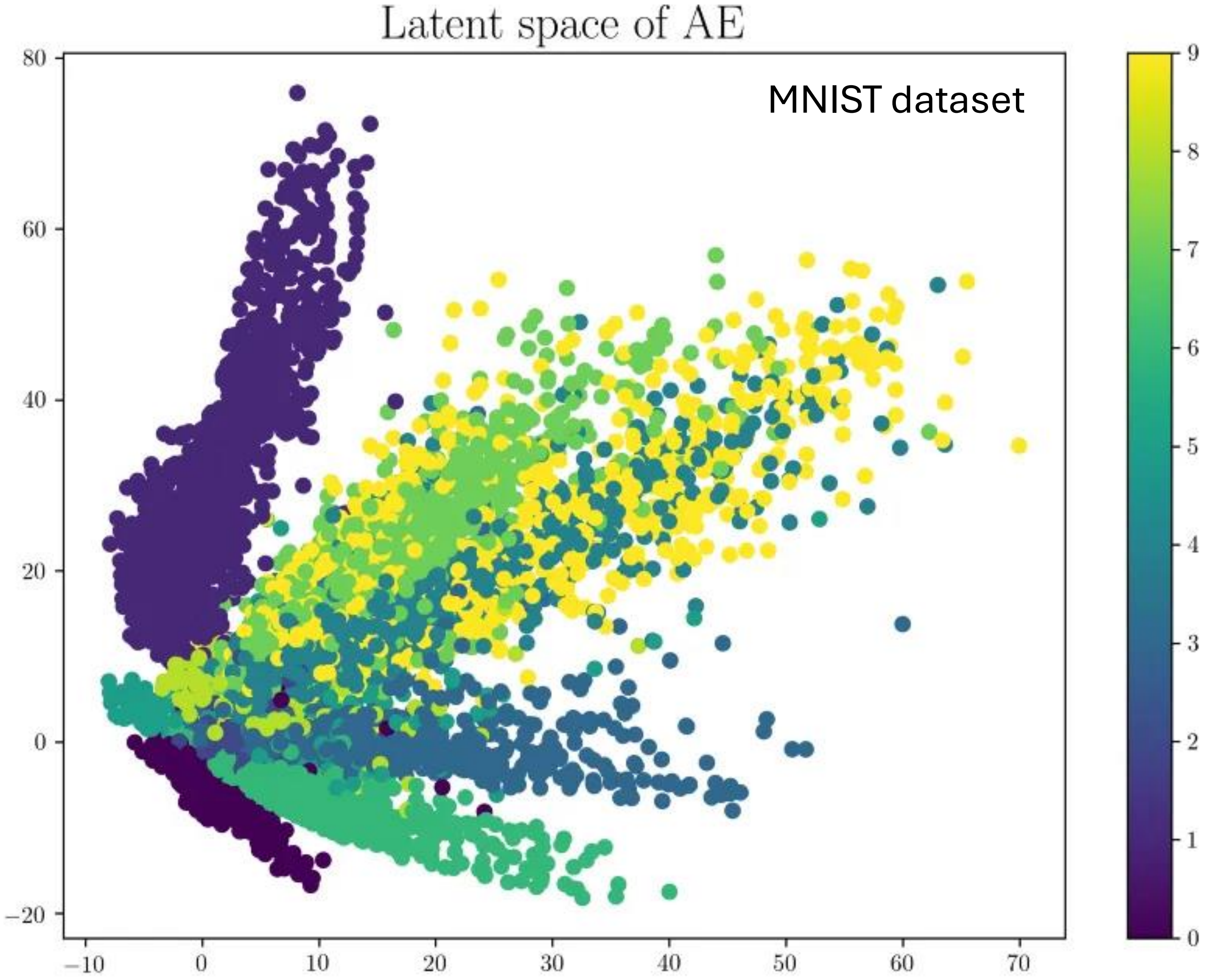
$\mu_{ref} = \frac{1}{N}\sum_{i=1}^{N} \delta_{x_i}$ $\quad d(x, x') = \|x - x'\|_2^2$

- Vanilla: $L(\theta, \phi) := \mathbb{E}_{x \sim \mu_{ref}} [d(x, D_\theta(E_\phi(x)))]$
- With regularizations:
  - Denoising: map noised data to data
    $$L(\theta, \phi) = \mathbb{E}_{x \sim \mu_X, T \sim \mu_T} [d(x, (D_\theta \circ E_\phi \circ T)(x))]$$
  - Contractive: small change in encoder output for small change in input
    Add $L_{contractive}(\theta, \phi) = \mathbb{E}_{x \sim \mu_{ref}} \|\nabla_x E_\phi(x)\|_F^2$
  - Sparsity regularization for overcomplete AEs: a way of compressing by deactivating neurons instead of imposing an explicit bottleneck
    Add $L_{sparsity}(\theta, \phi) = \mathbb{E}_{x \sim \mu_X} \left[\sum_{k \in 1:K} w_k s(\hat{\rho}_k, \rho_k(x))\right]$ where

    sparsity of layer k $\rho_k(x) = \frac{1}{n}\sum_{i=1}^{n} a_{k,i}(x)$ sum of activations

    $s(\rho, \hat{\rho}) = KL(\rho || \hat{\rho})$

Variational AE – completely regularizing the latent space



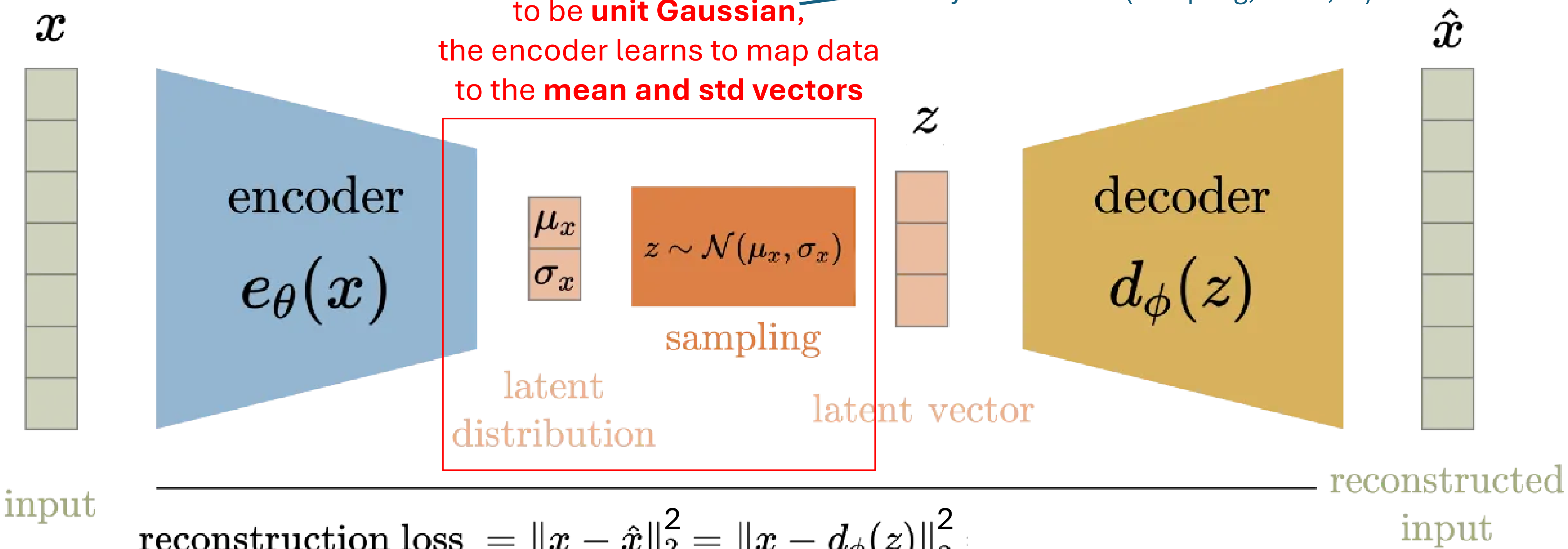
- Regions outside of the distribution cannot be used for data generation

- We must restrict ourselves within the distribution

- **Learn the distribution directly!**

Variational AE

force the latent distribution to be **unit Gaussian**, → easy to work with (sampling, math, …)
the encoder learns to map data to the **mean and std vectors**



$$\text{reconstruction loss} = \|x - \hat{x}\|_2^2 = \|x - d_\phi(z)\|_2^2$$

as desired

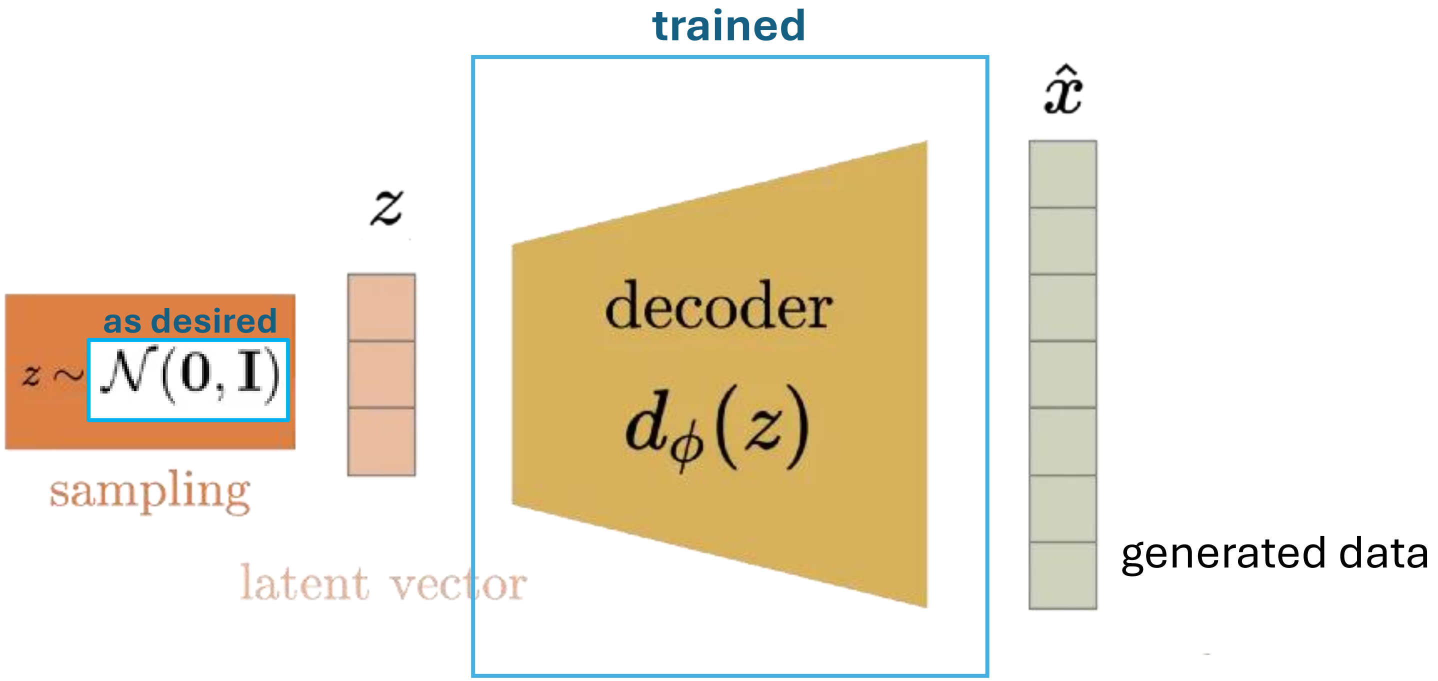
$$similarity\ loss = KL\ Divergence = D_{KL}(\mathcal{N}(\mu_x, \sigma_x) \parallel \mathcal{N}(\mathbf{0}, \mathbf{I}))$$

note: before training is done, each x will have its own Gaussian

$$loss = reconstruction\ loss + similarity\ loss$$

Variational AE

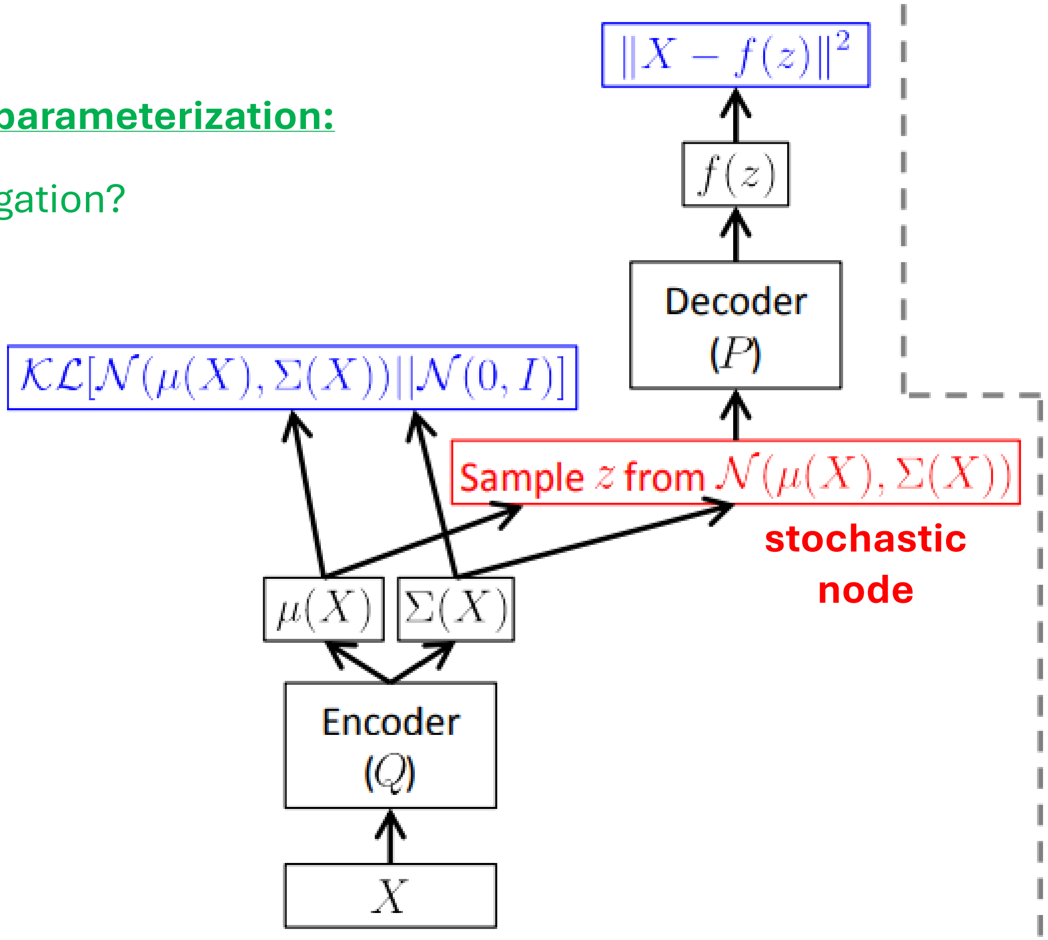
Data generator:



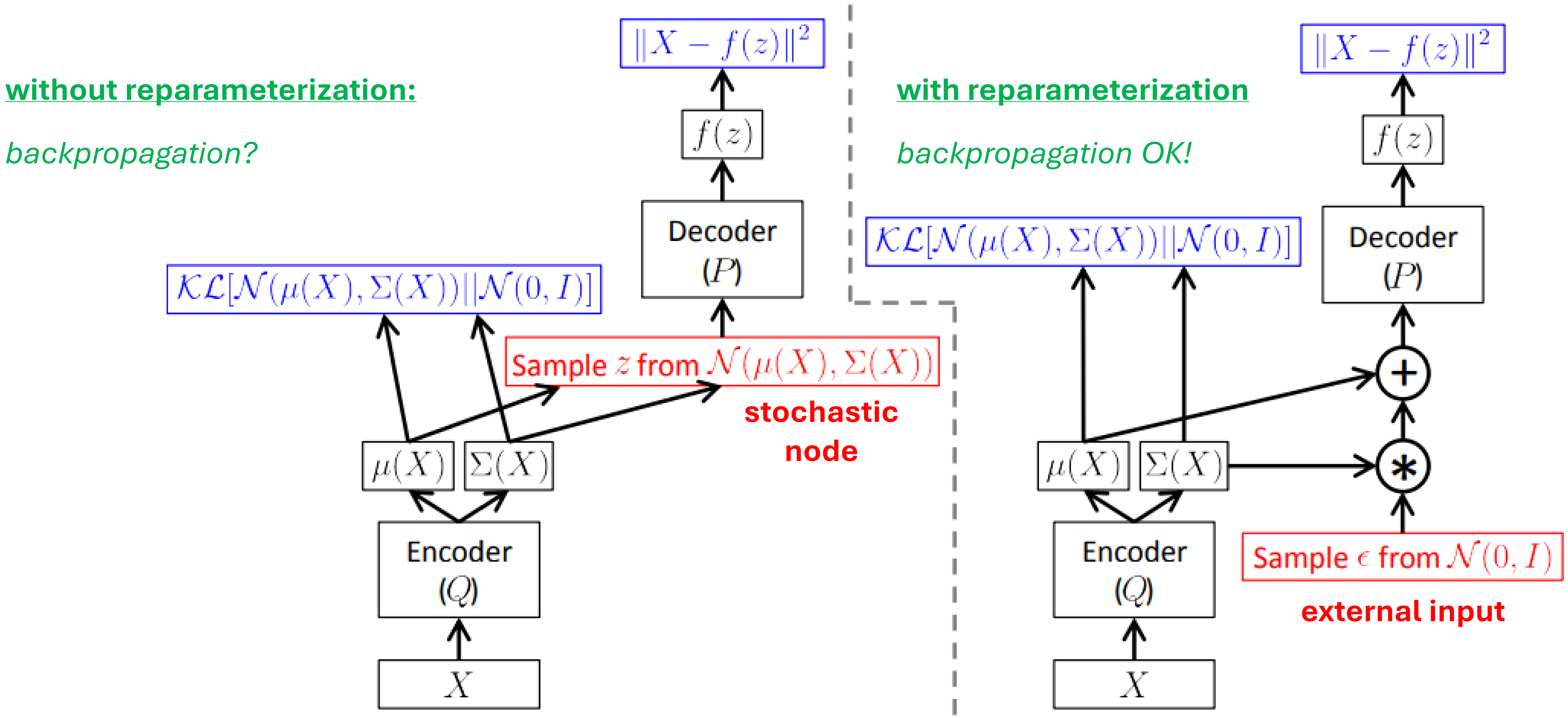
VAE – reparameterization trick

without reparameterization:

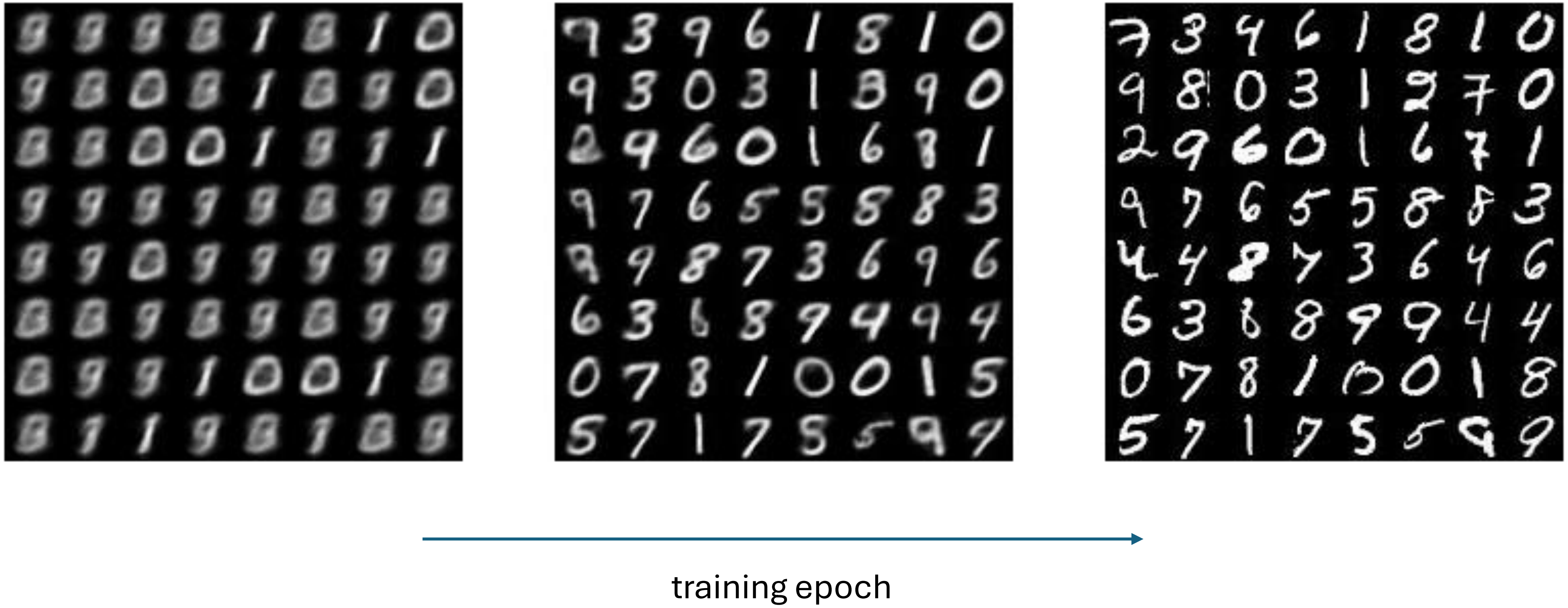
backpropagation?



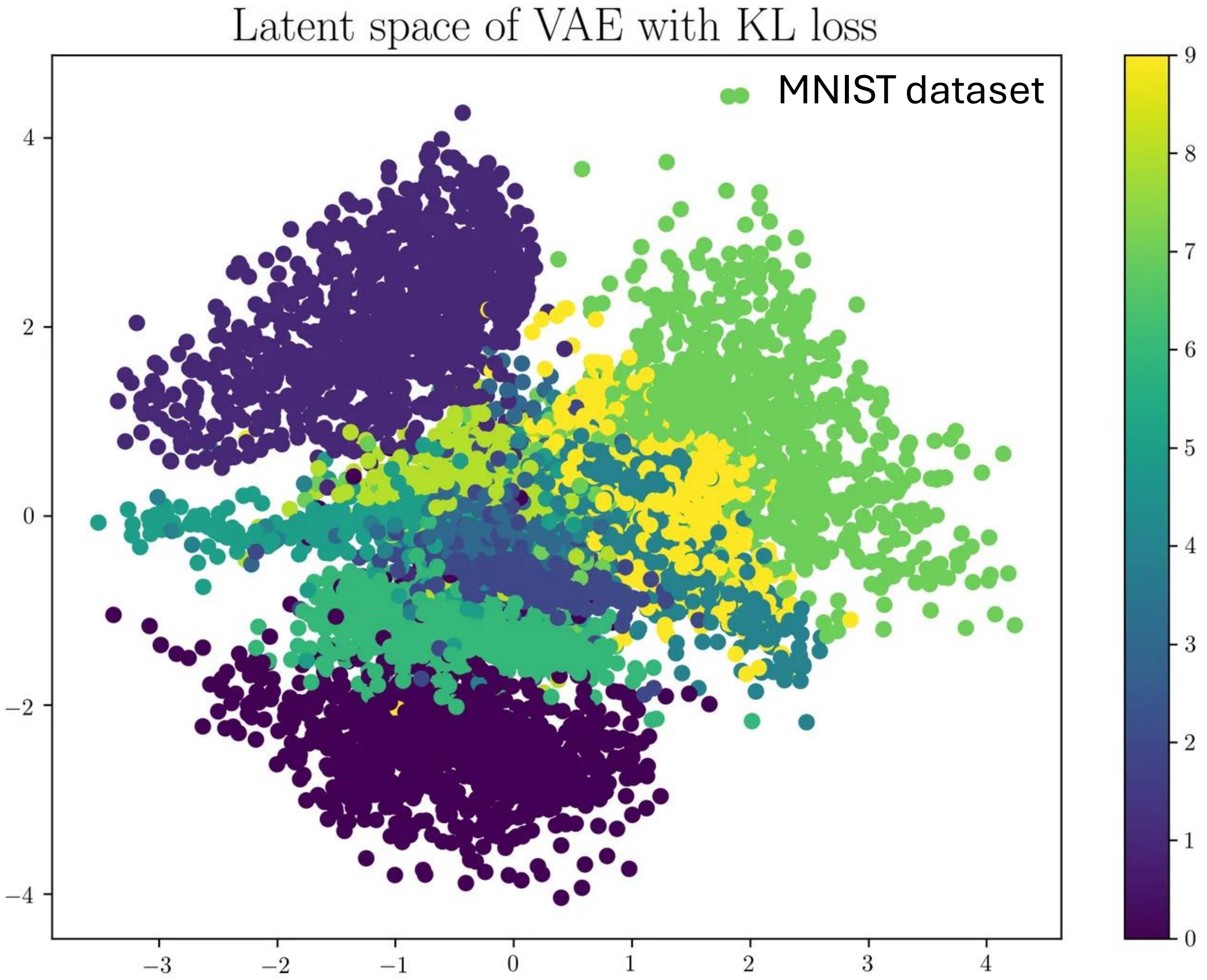
VAE – reparameterization trick



VAE – generated data examples



VAE – latent space



looks like a unit Gaussian
… more or less

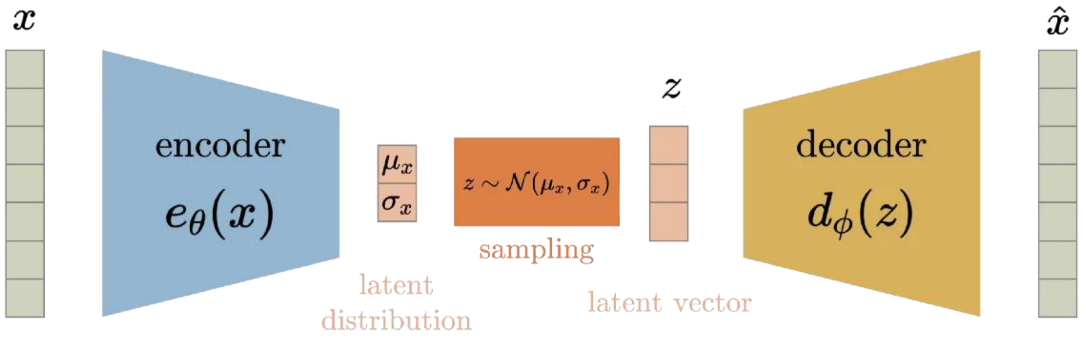
VAE – implementation

```python
class VAE(nn.Module):
    def __init__(self):
        super(VAE, self).__init__()

        self.fc1 = nn.Linear(784, 400)
        self.fc21 = nn.Linear(400, 20)
        self.fc22 = nn.Linear(400, 20)
        self.fc3 = nn.Linear(20, 400)
        self.fc4 = nn.Linear(400, 784)

    def encode(self, x):
        h1 = F.relu(self.fc1(x))
        return self.fc21(h1), self.fc22(h1)

    def reparametrize(self, mu, logvar):
        std = logvar.mul(0.5).exp_()
        if torch.cuda.is_available():
            eps = torch.cuda.FloatTensor(std.size()).normal_()
        else:
            eps = torch.FloatTensor(std.size()).normal_()
        eps = Variable(eps)
        return eps.mul(std).add_(mu)

    def decode(self, z):
        h3 = F.relu(self.fc3(z))
        return F.sigmoid(self.fc4(h3))

    def forward(self, x):
        mu, logvar = self.encode(x)
        z = self.reparametrize(mu, logvar)
        return self.decode(z), mu, logvar
```

```python
def loss_function(recon_x, x, mu, logvar):
    """
    recon_x: generating images
    x: origin images
    mu: latent mean
    logvar: latent log variance
    """
    BCE = reconstruction_function(recon_x, x)  # mse loss
    # loss = 0.5 * sum(1 + log(sigma^2) - mu^2 - sigma^2)
    KLD_element = mu.pow(2).add_(logvar.exp()).mul_(-1).add_(1).add_(logvar)
    KLD = torch.sum(KLD_element).mul_(-0.5)
    # KL divergence
    return BCE + KLD
```

```python
for epoch in range(num_epochs):
    model.train()
    train_loss = 0
    for batch_idx, data in enumerate(dataloader):
        img, _ = data
        img = img.view(img.size(0), -1)
        img = Variable(img)
        if torch.cuda.is_available():
            img = img.cuda()
        optimizer.zero_grad()
        recon_batch, mu, logvar = model(img)
        loss = loss_function(recon_batch, img, mu, logvar)
        loss.backward()
        train_loss += loss.data[0]
        optimizer.step()
        if batch_idx % 100 == 0:
            print('Train Epoch: {} [{}/{} ({:.0f}%)]\tLoss: {:.6f}'.format(
                epoch,
                batch_idx * len(img),
                len(dataloader.dataset), 100. * batch_idx / len(dataloader),
                loss.data[0] / len(img)))
```

VAE – a Bayesian understanding



1. We want to generate data from the distribution $p(X)$
   - We only have samples (training data), hard to guess a formula for sampling

2. In VAE the data generator is the decoder, and we decide to sample the latent distribution $p(Z)$
   - We can write $p(X) = \sum_Z p(X|Z)p(Z)$ = decoder • latent distribution

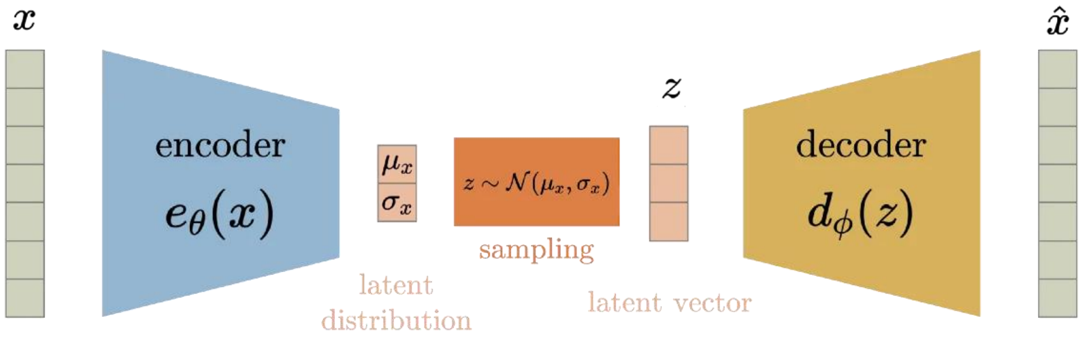
     we want this to be easy to sample

3. The encoder generates the latent variable. In terms of probability, the encoder is $p(Z|X)$ = encoder = encoder's posterior given the input X

   we fix a parameterization of the posterior, and have the encoder spit out the parameters according to input

4. Now think about what happens if we train only with reconstruction loss

VAE – a Bayesian understanding



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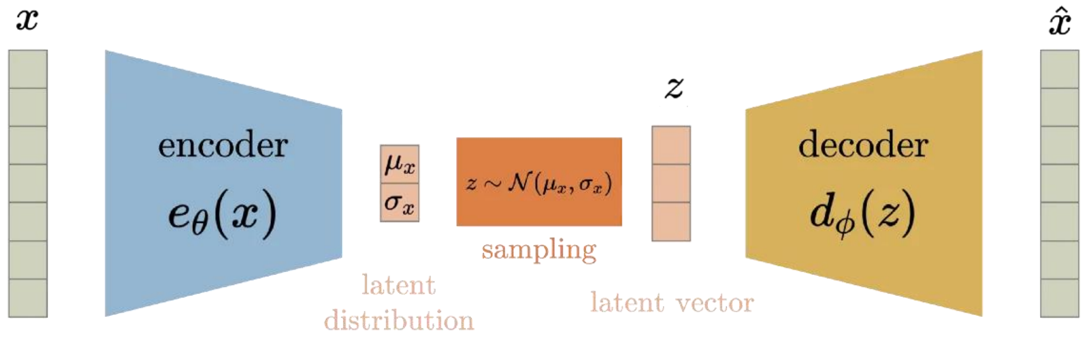
4. Now think about what happens if we train only with reconstruction loss

   the encoder will learn to be "deterministic" by, e.g., setting std to zero! ➔ just an AE!

VAE – a Bayesian understanding



$p(Z|X)$ = encoder

$p(X) = \sum_Z p(X|Z)p(Z)$ = decoder • latent distribution

Gaussian is a simple choice; a uniform distribution probably won't work

$$D_{KL}(\mathcal{N}(\mu_x, \sigma_x) \parallel \mathcal{N}(\mathbf{0}, \mathbf{I}))$$

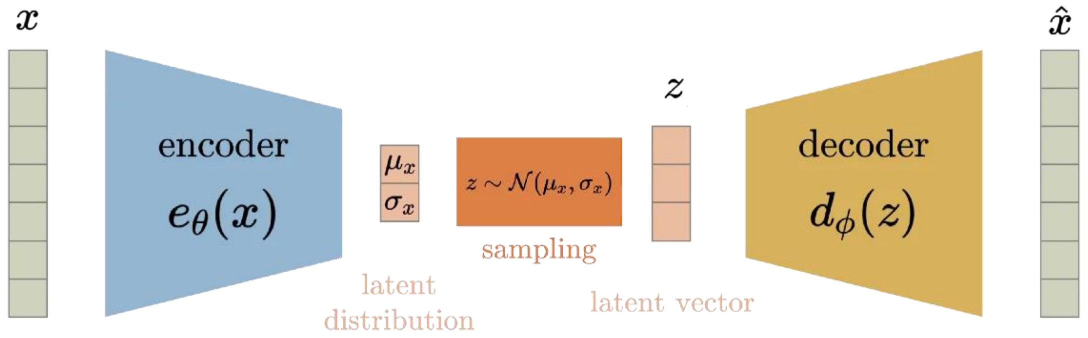
for any X

- The solution is to fix $p(Z|X)$ = $\mathcal{N}(0, I)$ by the similarity loss

- This is great, because:
  - $p(Z) = \sum_X p(Z|X)p(X) = \sum_X \mathcal{N}(0,I)p(X) = \mathcal{N}(0,I)\sum_X p(X) = \mathcal{N}(0,I)$

    is indeed what we plan to sample *Z* from

VAE – a Bayesian understanding



- And the training dynamics is right
  - The reconstruction loss is counteracting the similarity loss!

reconstruction loss > similarity loss
learning ➔ reconstruction loss ↓ + similarity loss ↑
[lower the std (increase KL) makes it easier to reconstruct]

similarity loss > reconstruction loss
learning ➔ similarity loss ↓ + reconstruction loss ↑
[increase the std makes it harder to reconstruct]

reconstruction loss hates noise (std); similarity loss wants noise

generative aspect