

CPEN 455: Deep Learning

Lecture 10: Autoencoders, Denoising Autoencoders, and Variational Autoencoders

Original slides by **Renjie Liao**

Presented by **Qihang Zhang**

University of British Columbia

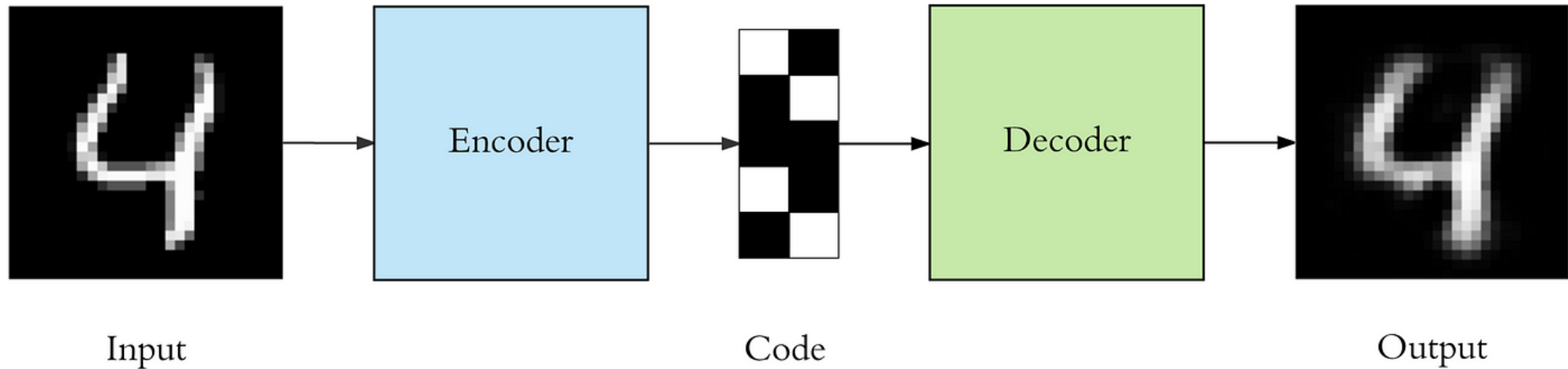
Winter, Term 2, 2024

Outline

- Autoencoders
 - **Motivation & Overview**
 - Linear Autoencoders & PCA
 - Deep Autoencoders
- Denoising Autoencoders
- Variational Autoencoders
 - Motivation & Overview
 - Evidence Lower Bound (ELBO)
 - Models
 - Amortized Inference
 - Reparameterization Trick

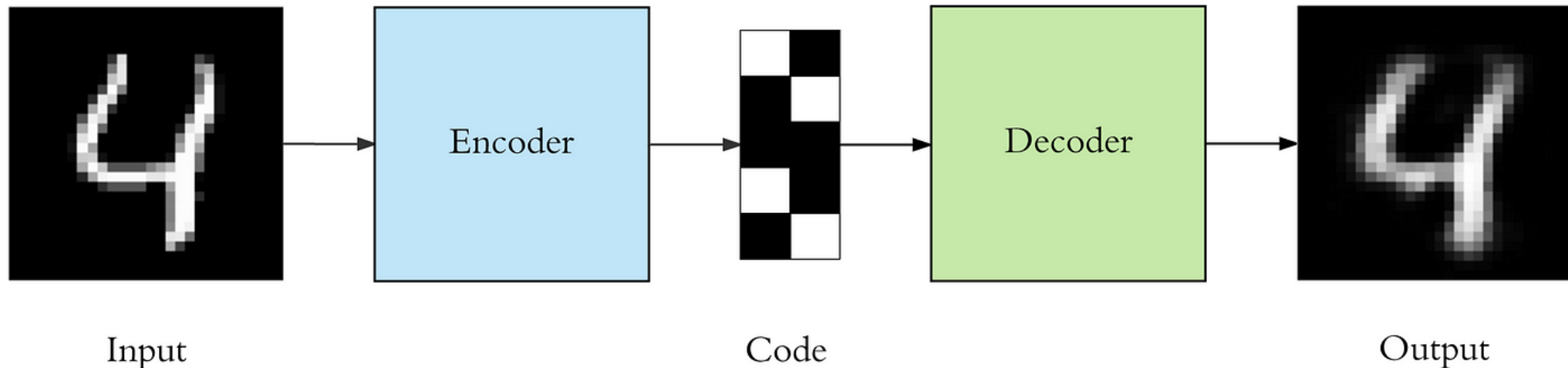
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- Autoencoders are feed-forward neural networks that reconstruct/predict the input



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- To make it non-trivial, we need a *bottleneck* (i.e. the dimension of code being much smaller compared to the input). (explain later).



Autoencoders (AEs)

Why should we care?

- Dimension reduction

e.g., visualizing high-dimension data

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- Unsupervised representation learning

e.g., if we have abundant data without annotations, learned representations will potentially be useful for downstream tasks like classification and regression

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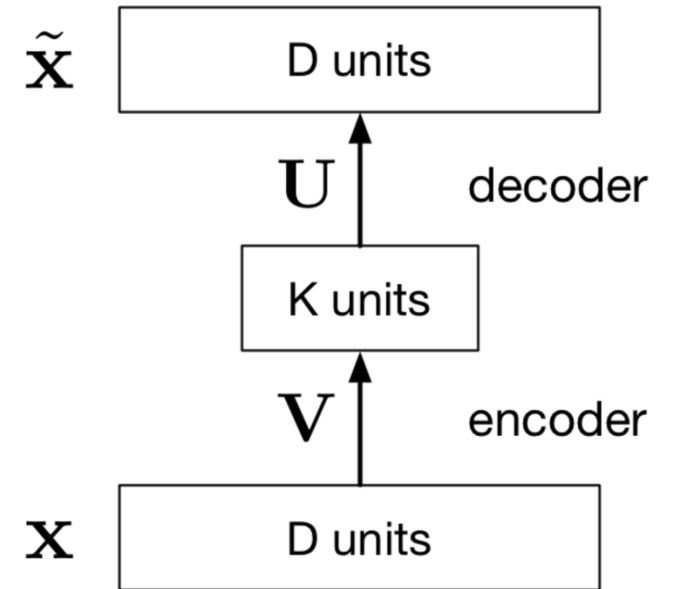
Linear Autoencoders

Simplest autoencoders: a single hidden layer with linear activations

We can train them by minimizing the mean squared errors (MSE):

$$\ell(\tilde{\mathbf{x}}, \mathbf{x}) = \|\tilde{\mathbf{x}} - \mathbf{x}\|_2^2$$

The network is $\tilde{\mathbf{x}} = UV\mathbf{x}$



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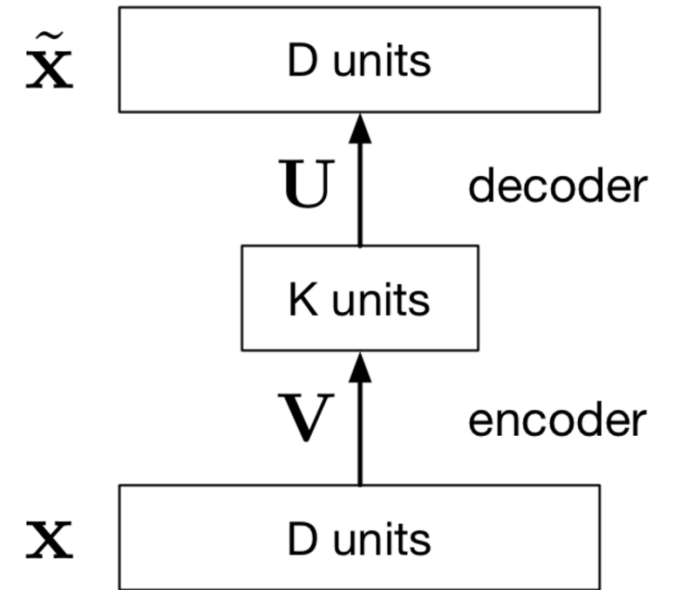
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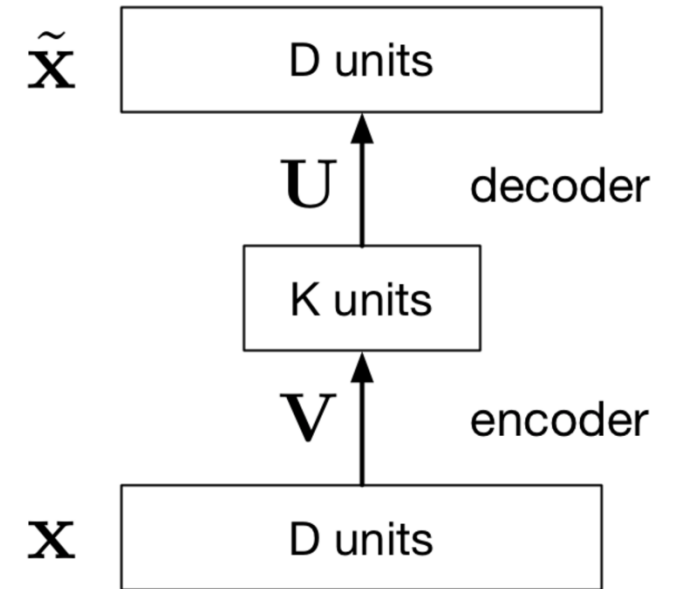
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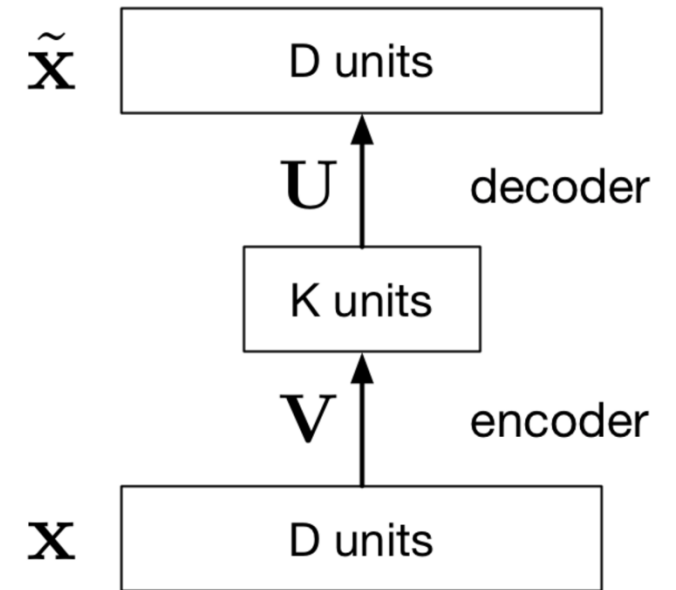
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$$\tilde{\mathbf{x}} = U^{D \times K} \mathbf{y} = [\vec{u}_1, \vec{u}_2, \dots, \vec{u}_K] \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_k \end{pmatrix} = \sum_{i=1}^K y_i \vec{u}_i$$
$$\mathbf{y} = V^{K \times D} \mathbf{x}$$



Linear Autoencoders & Principle Component Analysis

We know linear autoencoders map D -dimensional input to a K -dimensional subspace

What is the best possible K -dimensional mapping?

The one that minimizes the reconstruction error!

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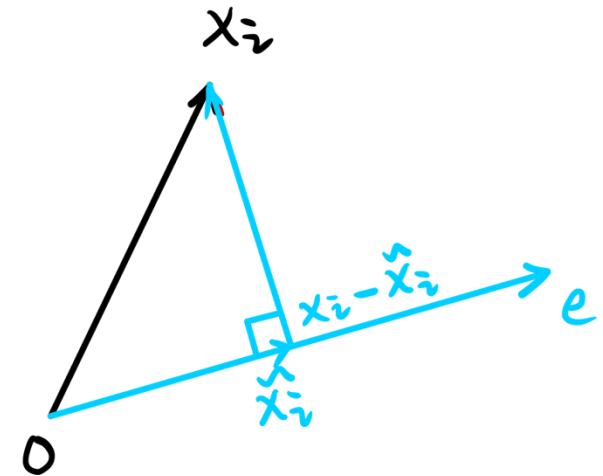
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Consider $D=2$ $K=1$



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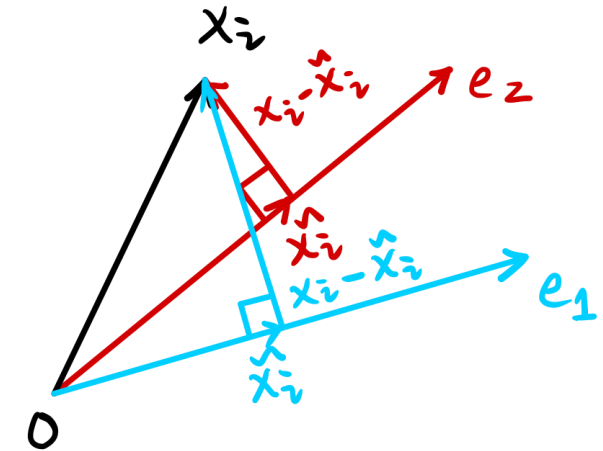
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$$\|\mathbf{x}_i\|^2 = \|\hat{\mathbf{x}}_i\|^2 + \|\tilde{\mathbf{x}}_i\|^2$$

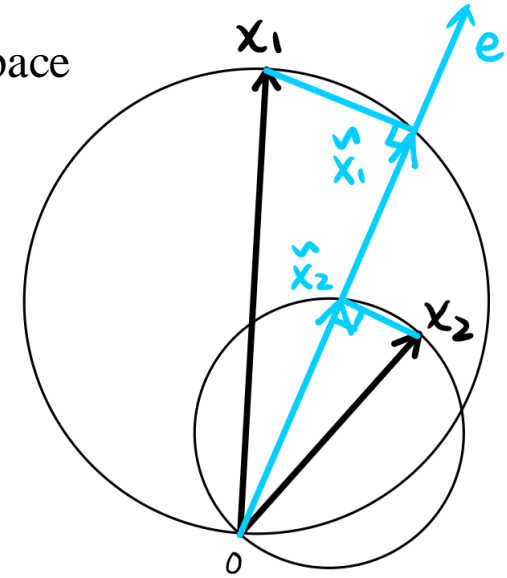
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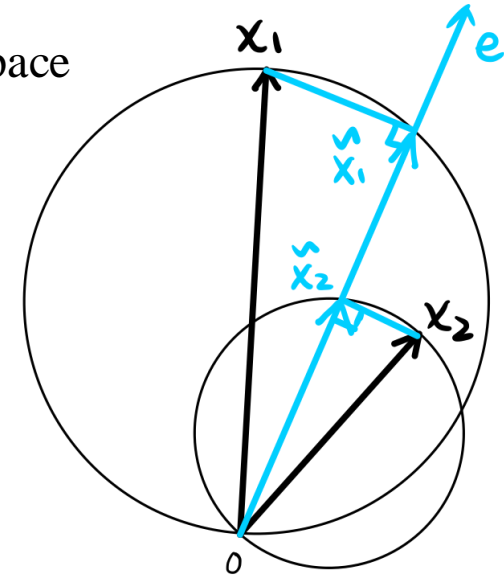
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To obtain it, let us first center the data, i.e., $\tilde{\mathbf{x}}_i = \mathbf{x}_i - \frac{1}{N} \sum_{i=1}^N \mathbf{x}_i$

By Pythagorean Theorem, we have:

$$\underbrace{\frac{1}{N} \sum_{i=1}^N \|\mathbf{x}_i\|^2}_{\text{constant}} = \underbrace{\frac{1}{N} \sum_{i=1}^N \|\mathbf{x}_i - \tilde{\mathbf{x}}_i\|^2}_{\text{reconstruction error}} + \underbrace{\frac{1}{N} \sum_{i=1}^N \|\tilde{\mathbf{x}}_i\|^2}_{\text{projected variance}}$$

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Maximizing the projected variance is equivalent to minimizing the reconstruction error!

You can maximize the variance in closed-form via *principle component analysis (PCA)*!

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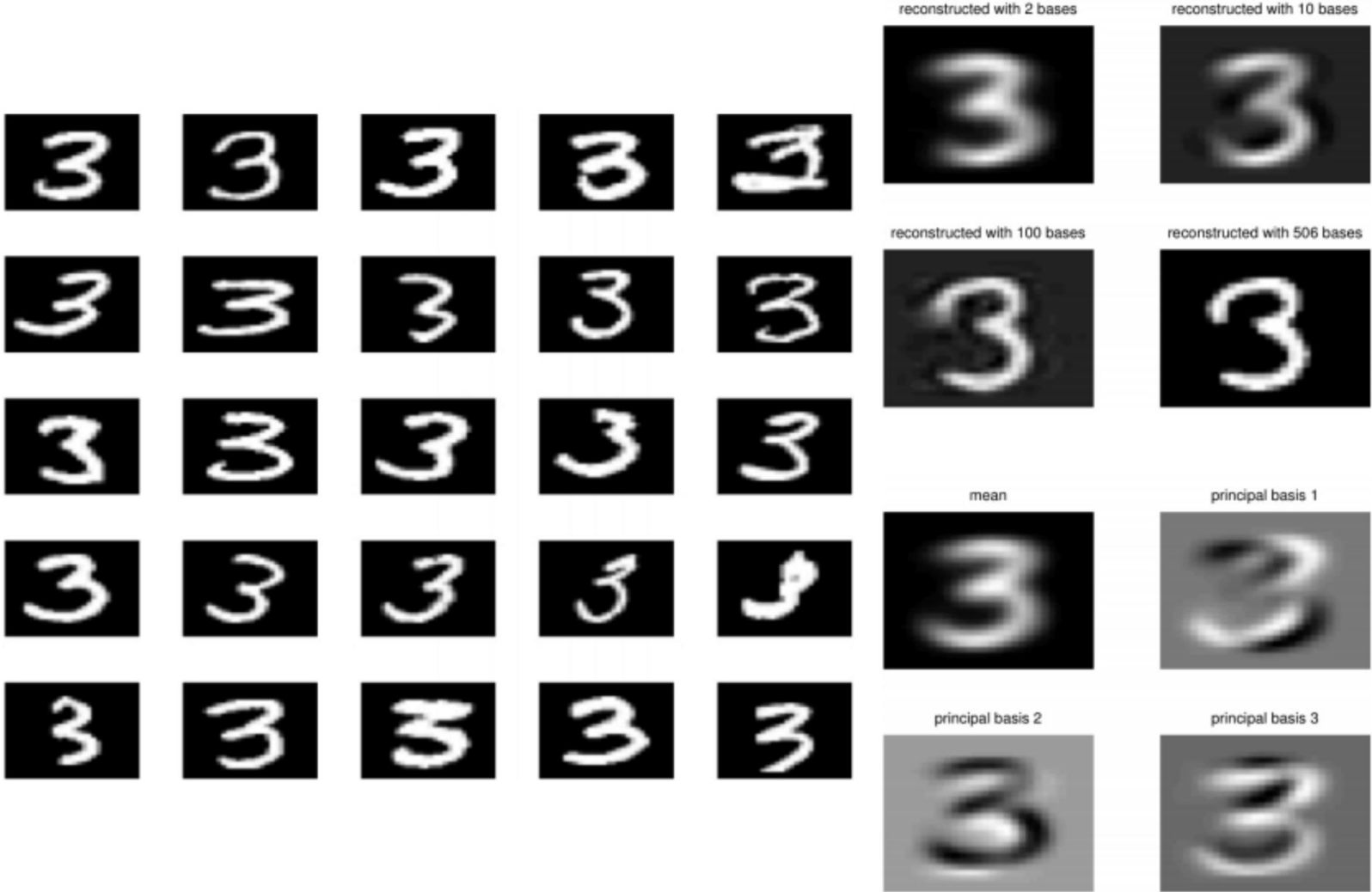
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Principle components of faces (“Eigenfaces”) from CBCL dataset:



Linear Autoencoders & Principle Component Analysis

Principle components of digits from MNIST dataset:



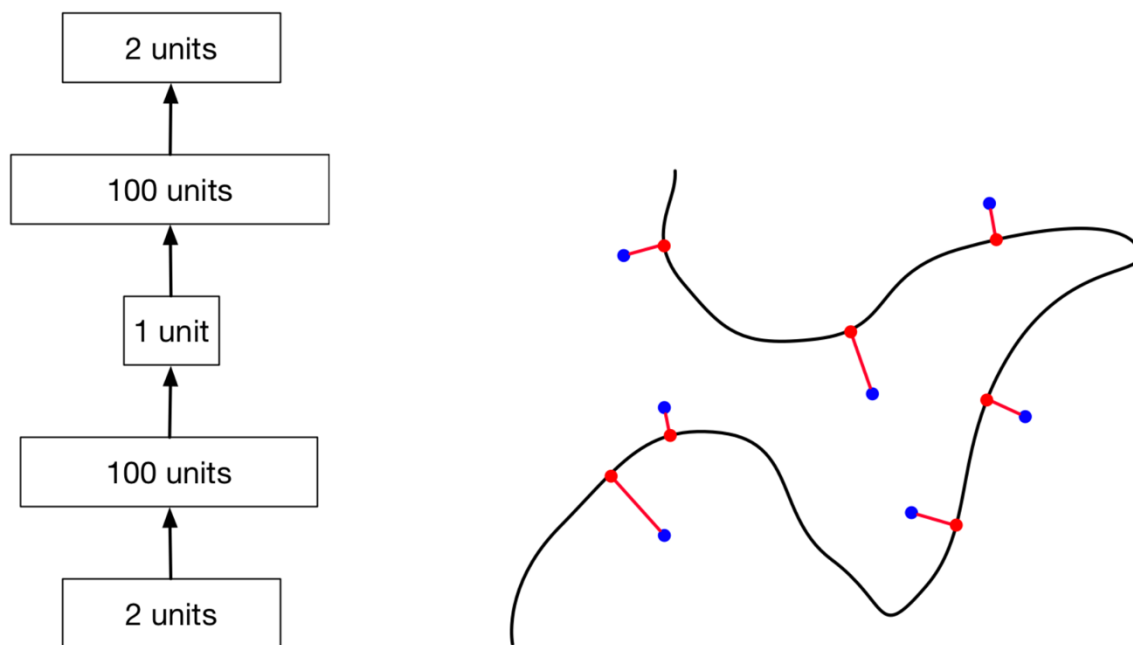
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Deep Autoencoders

Deep autoencoders learn to project data onto a *manifold* instead of a subspace

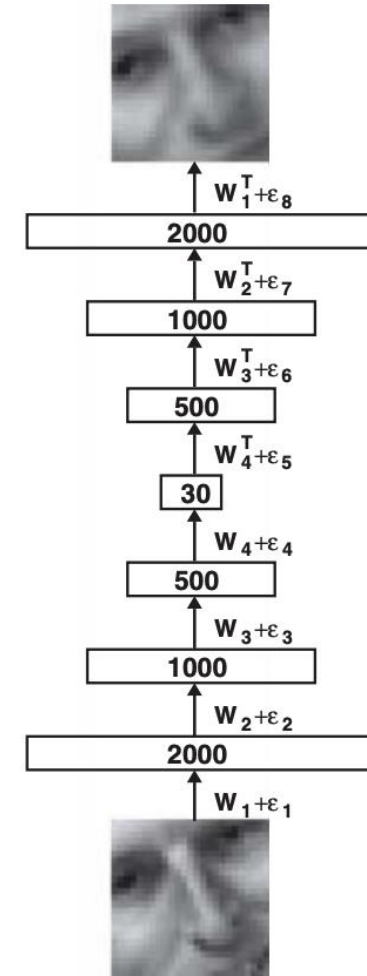
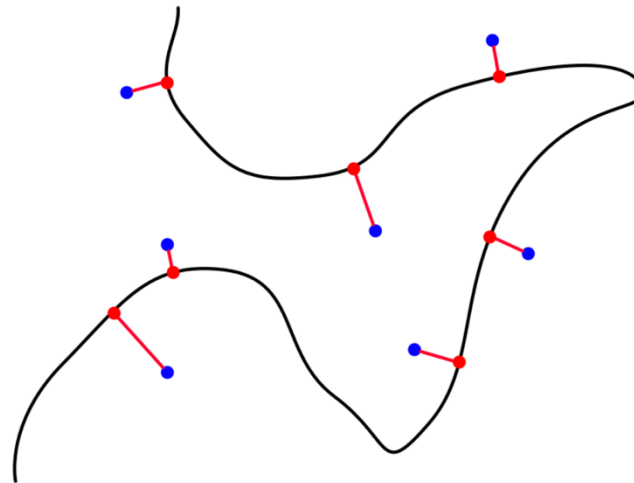
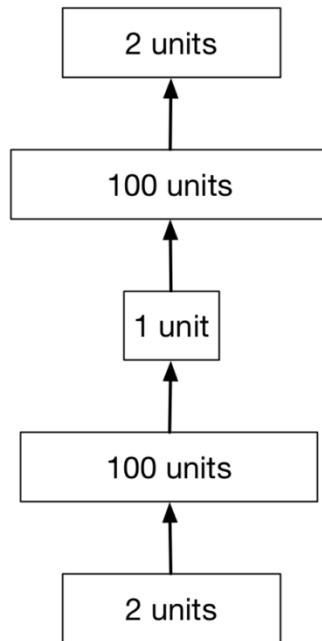
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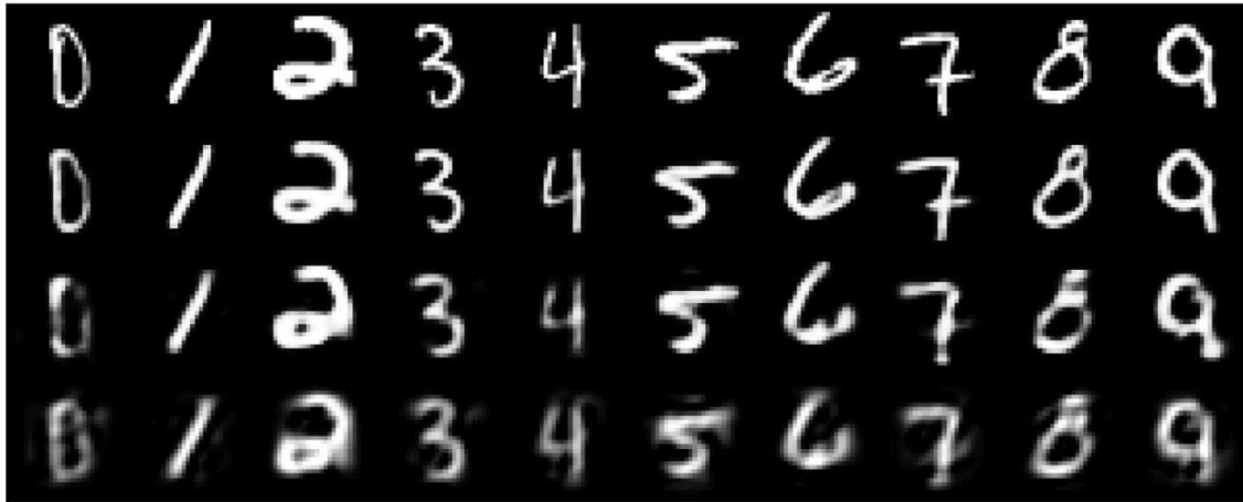
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Deep autoencoders can learn more powerful codes/representations compared to linear ones (PCA)

Reconstructions with various methods on MNIST dataset:



Real data

30-d deep autoencoder

30-d logistic PCA

30-d PCA

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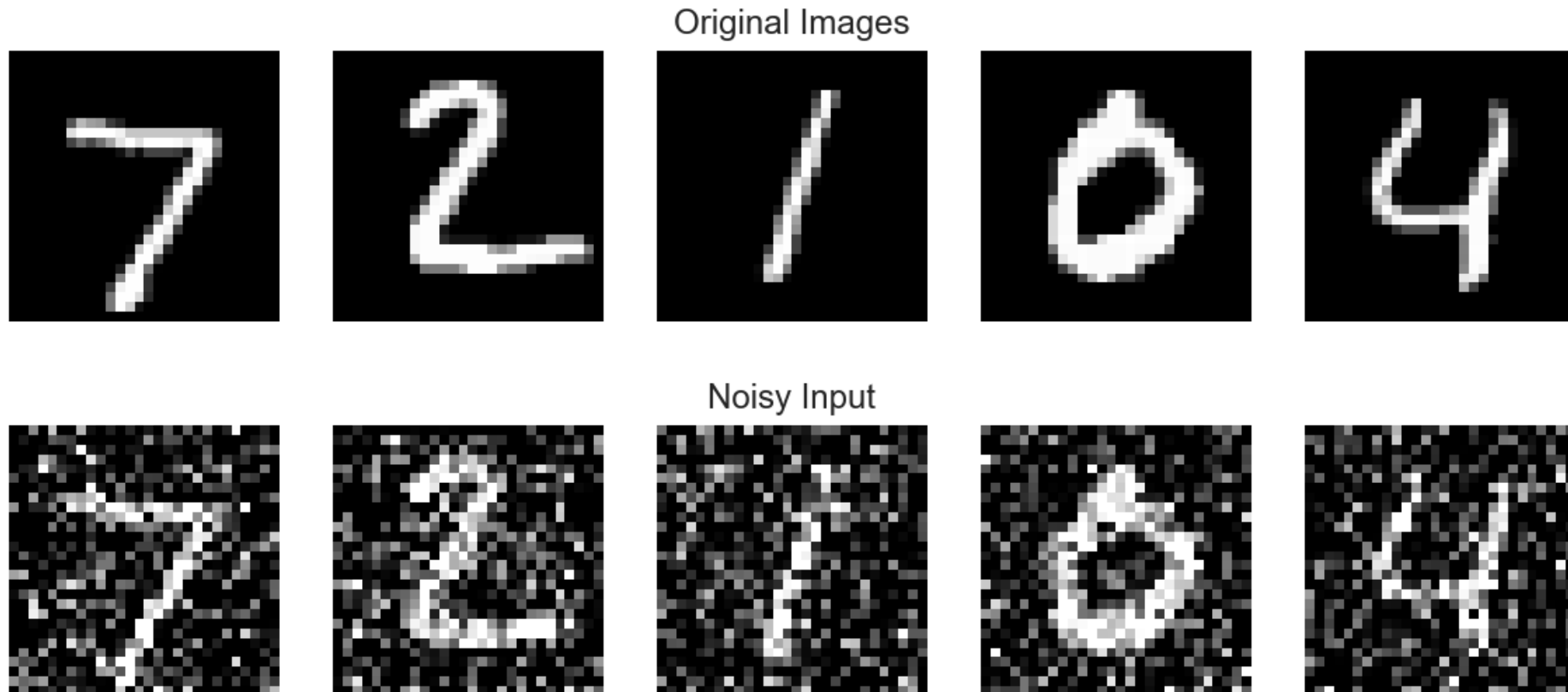
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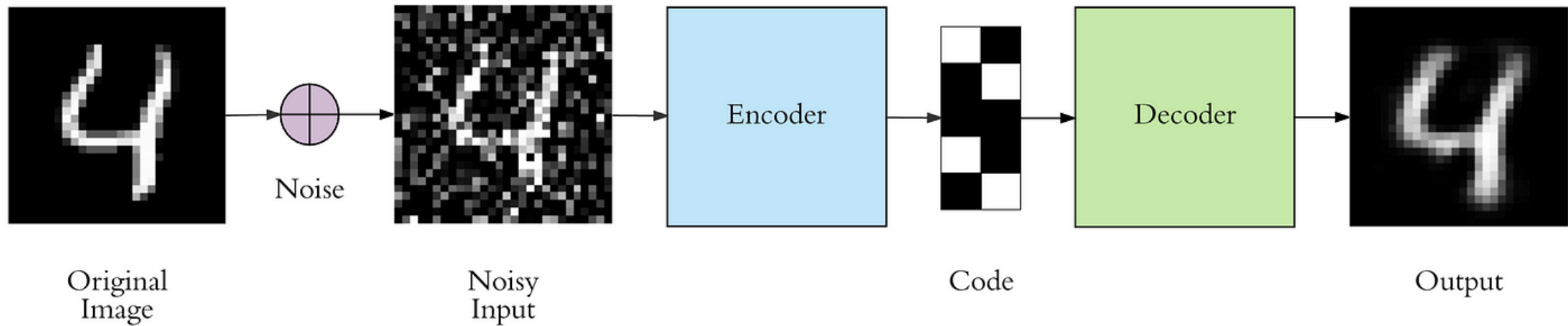


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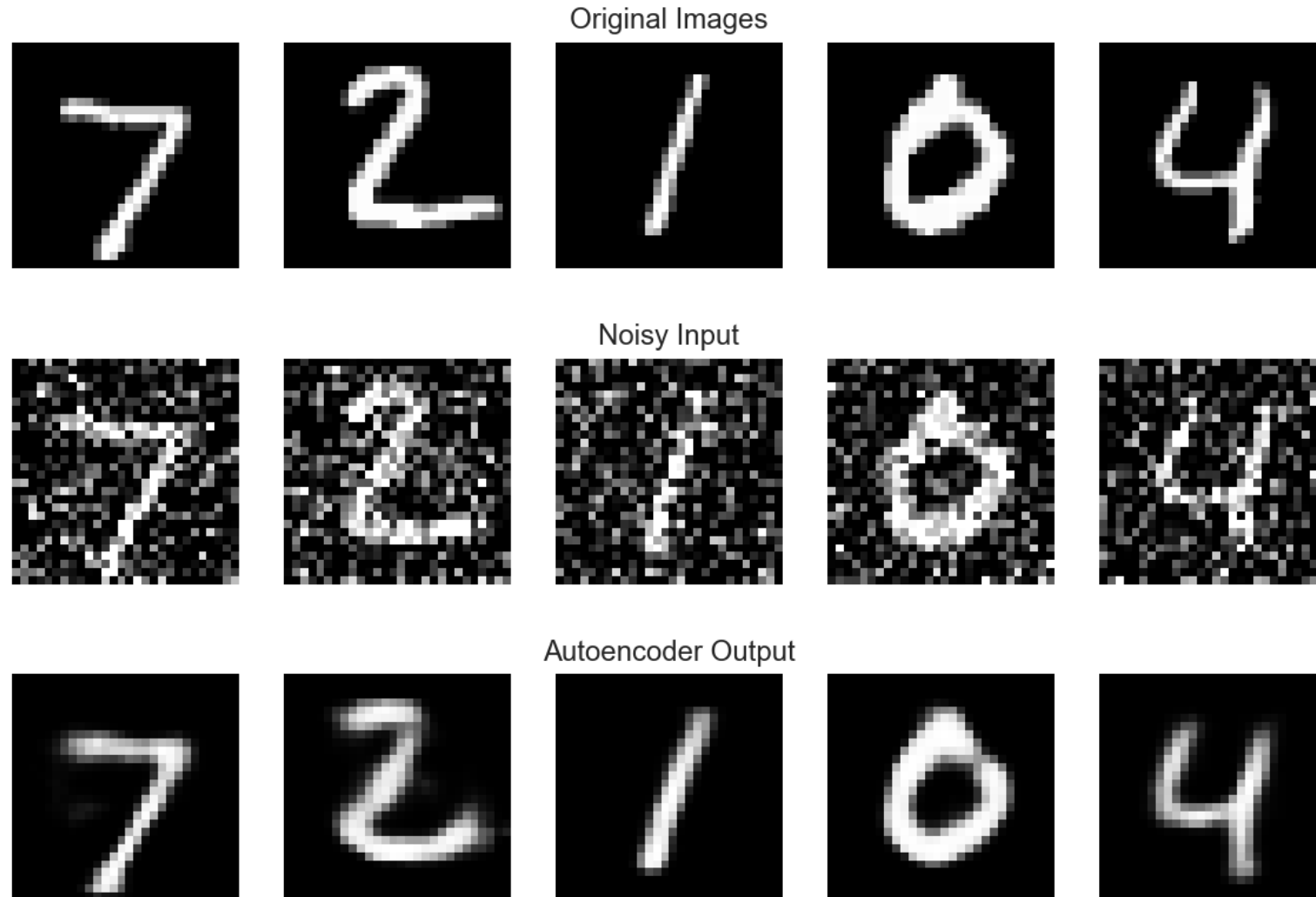
We can also achieve a similar goal via **denoising**!

We add random noise (e.g., additive Gaussian) and force the neural network to learn useful representations so that *structures in images are preserved whereas noise is removed!*



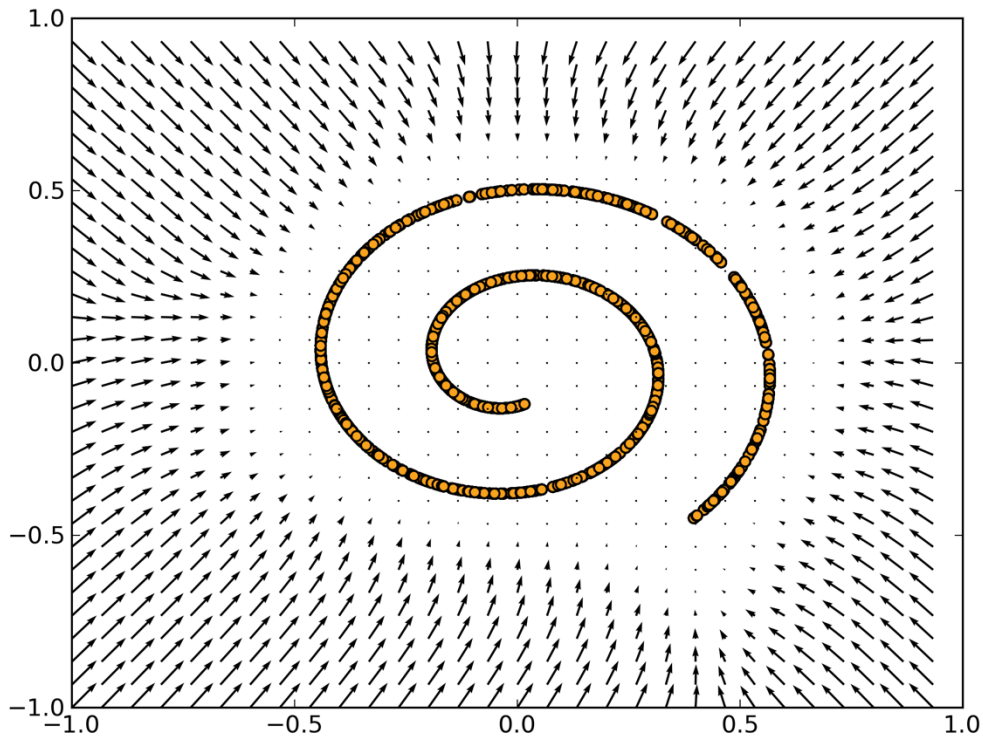
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DAEs can do a great job in denoising:

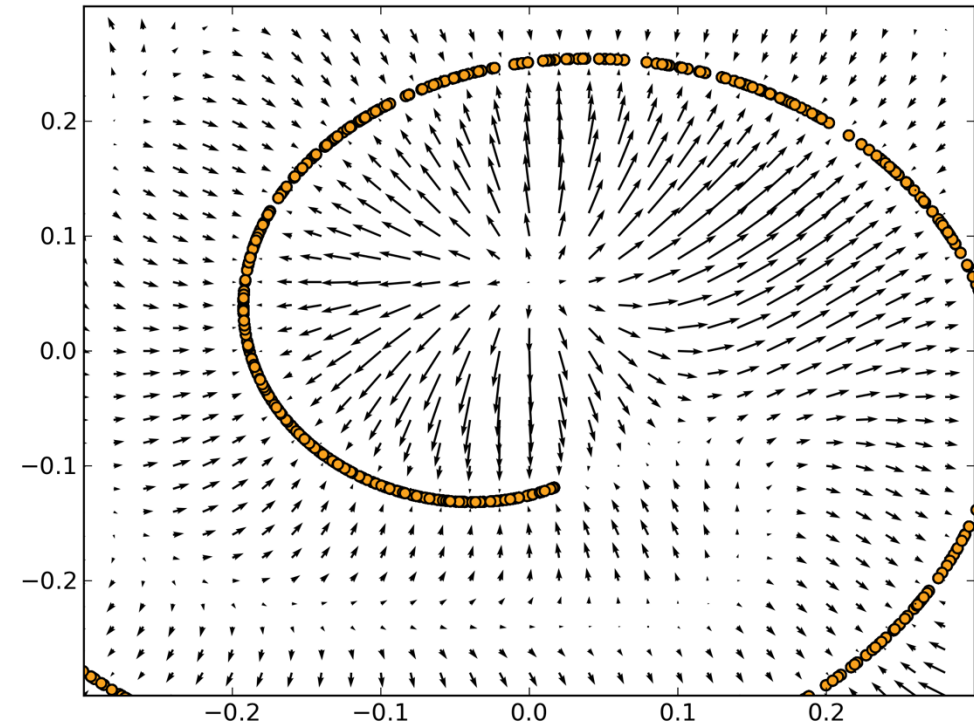


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DAEs can learn correct vector fields (reconstruction – noisy input) that point to data manifold (spiral):



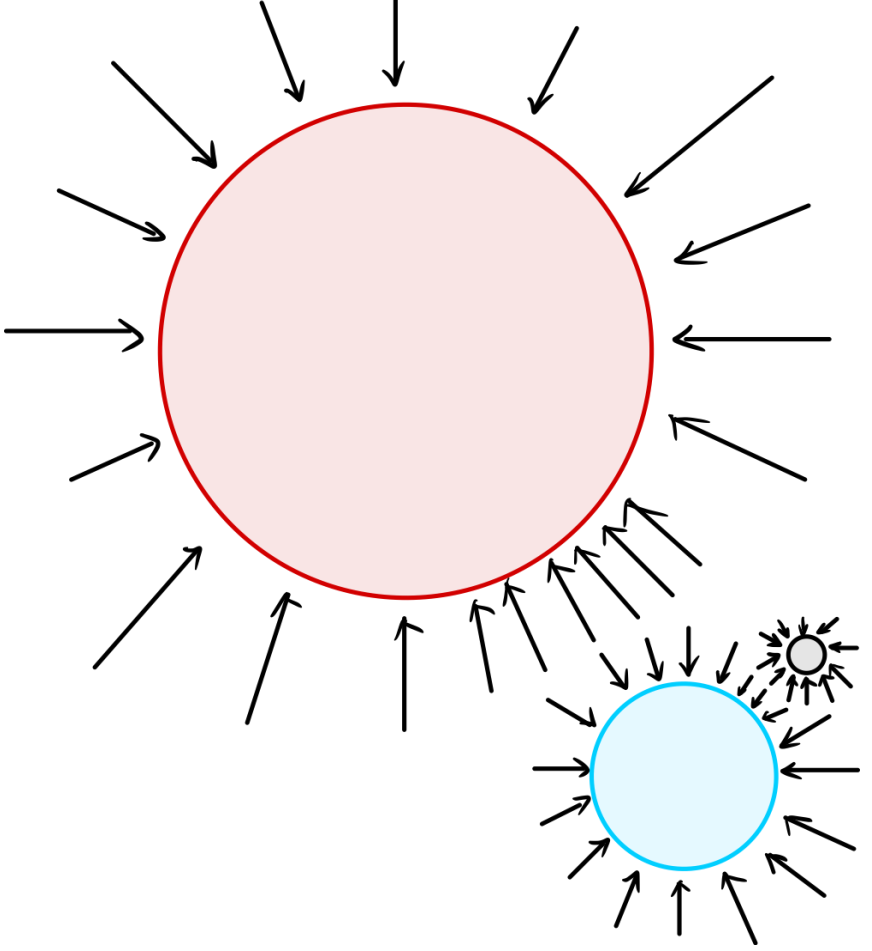
zoom out



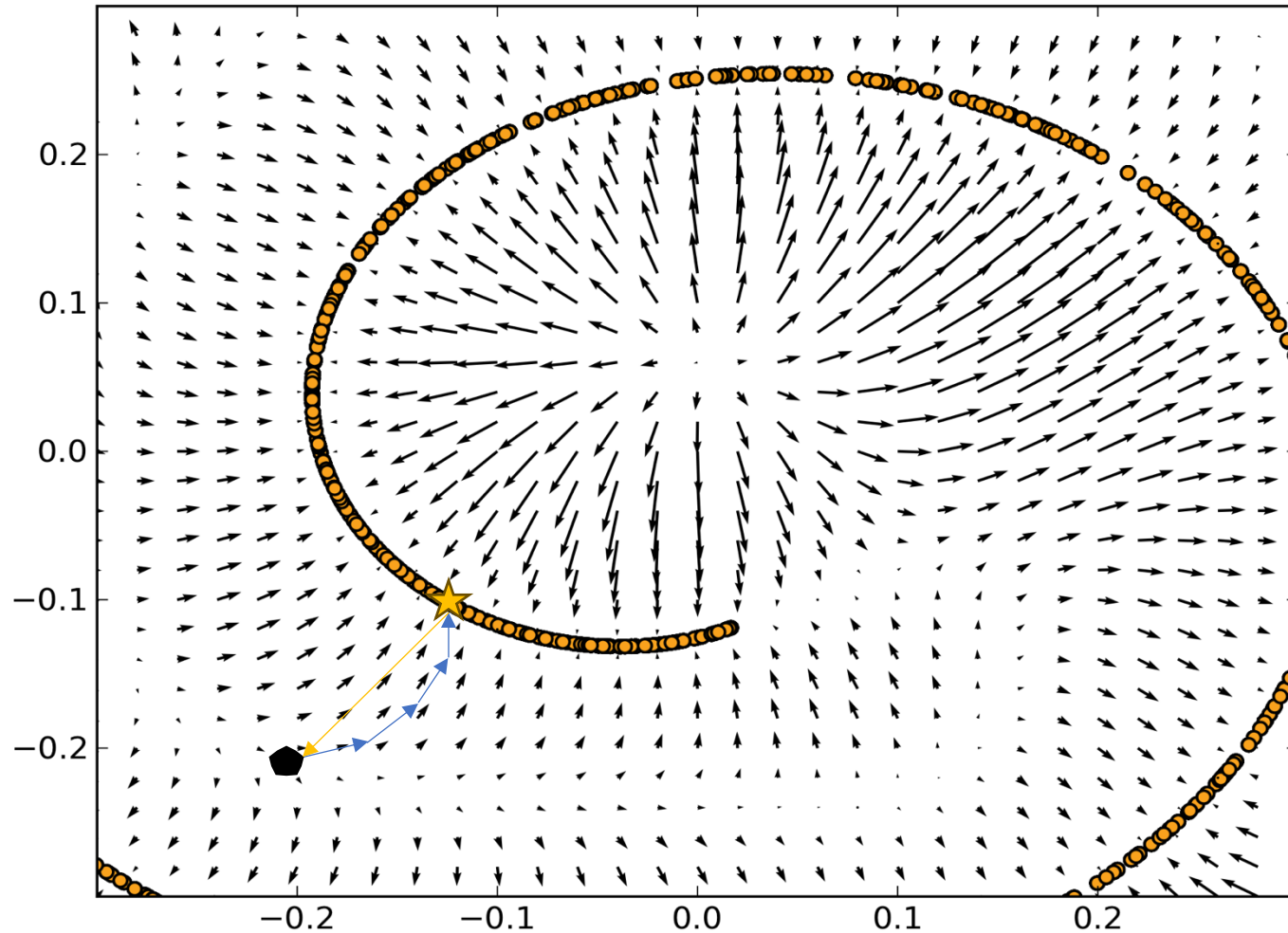
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Reminder:

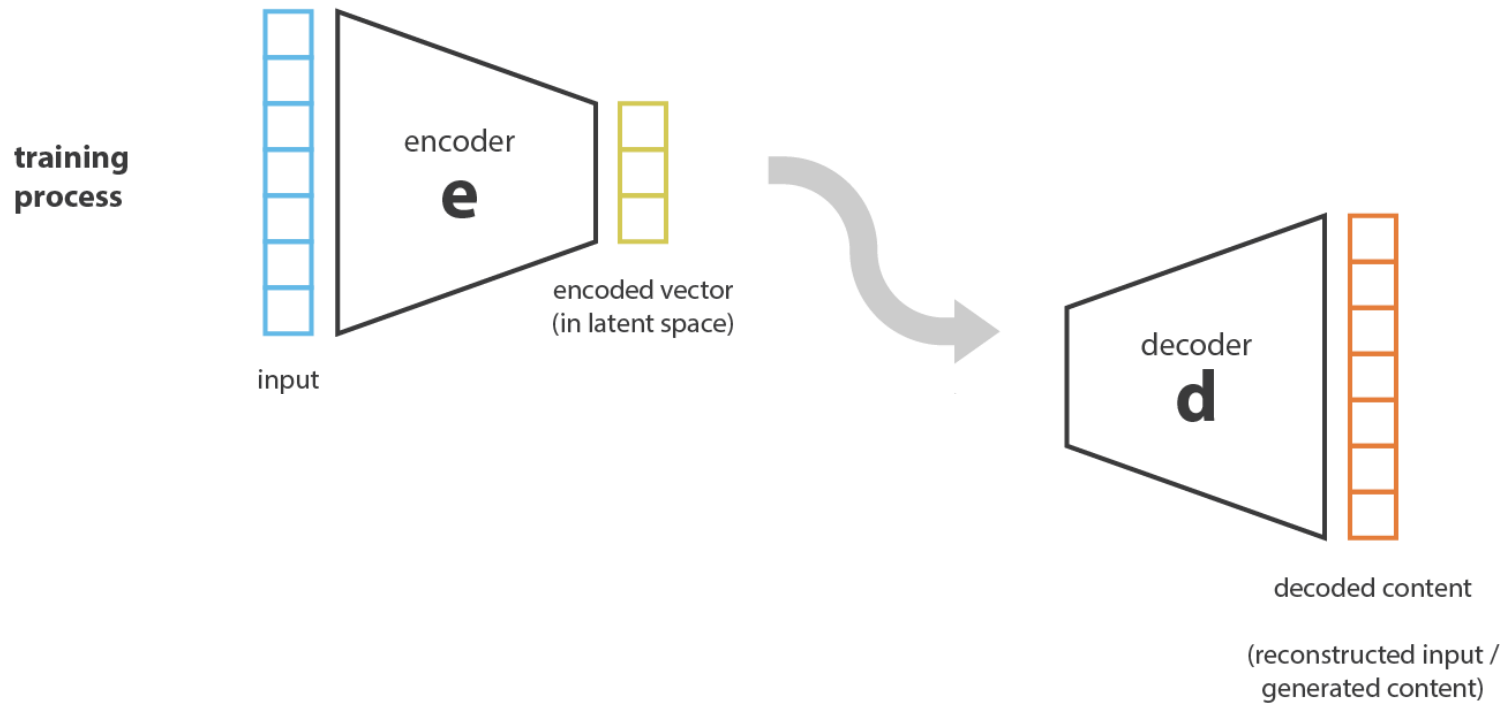
Please start the course project as soon as possible.

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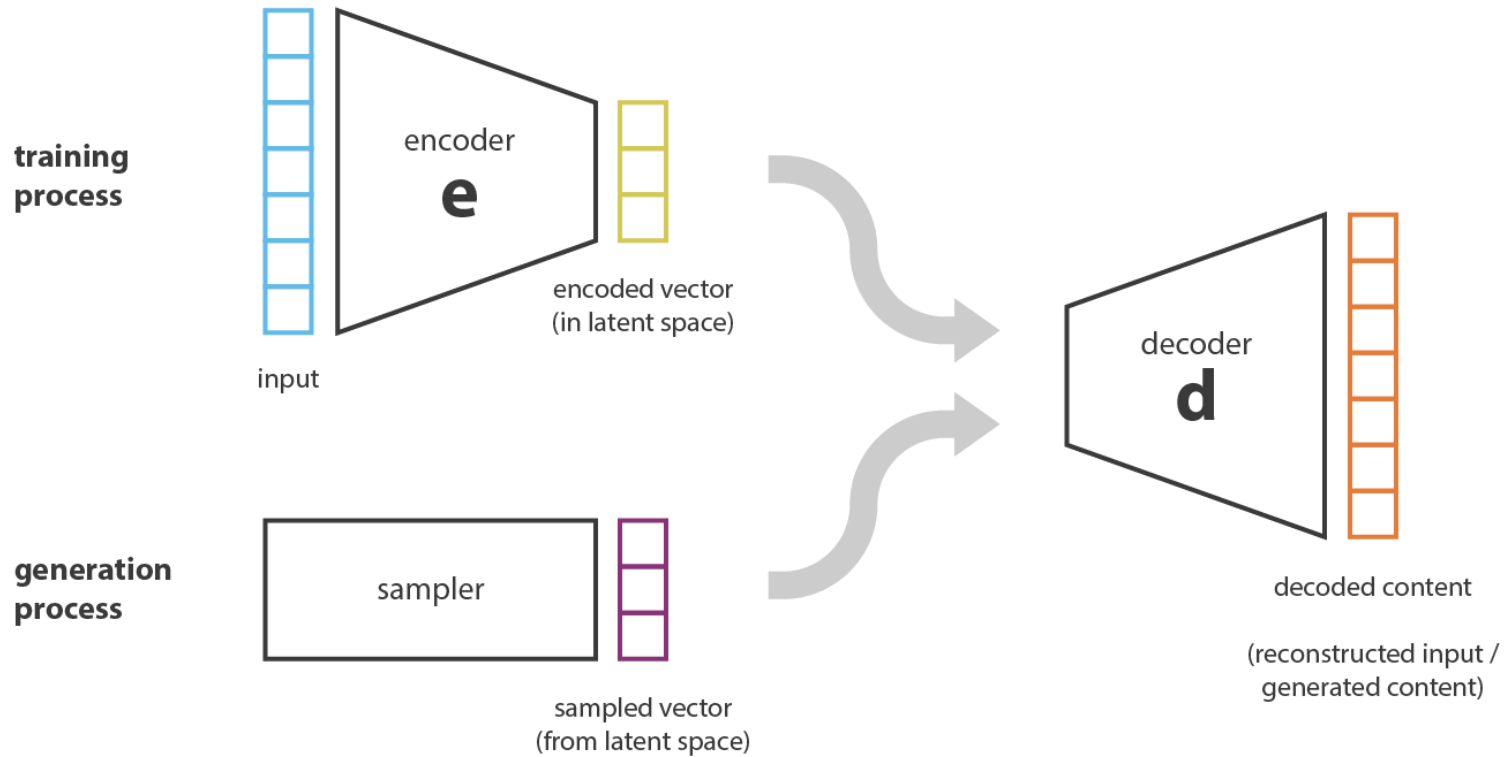
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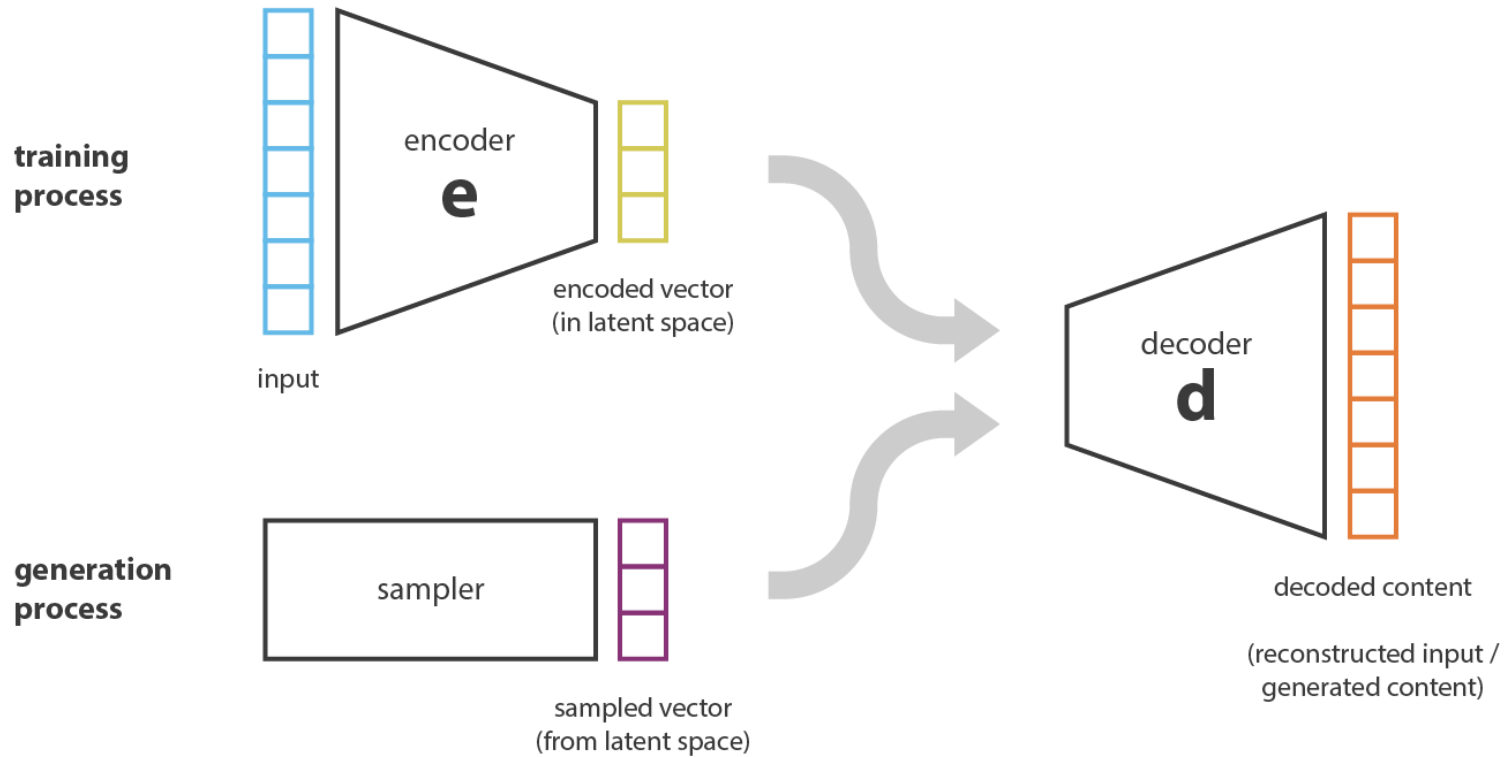
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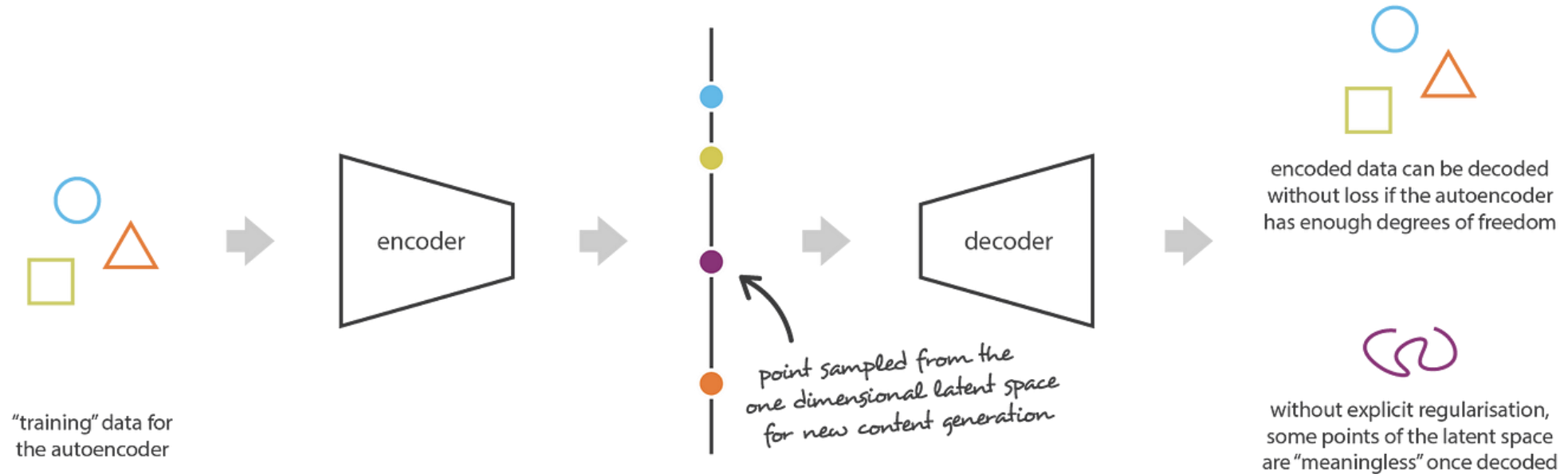
What would happen?



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What would happen? *Sampled data could be very bad if sampled latent codes are far off the manifold!*



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Ideally, we hope to learn a regular latent space that similar latent codes generate similar data!

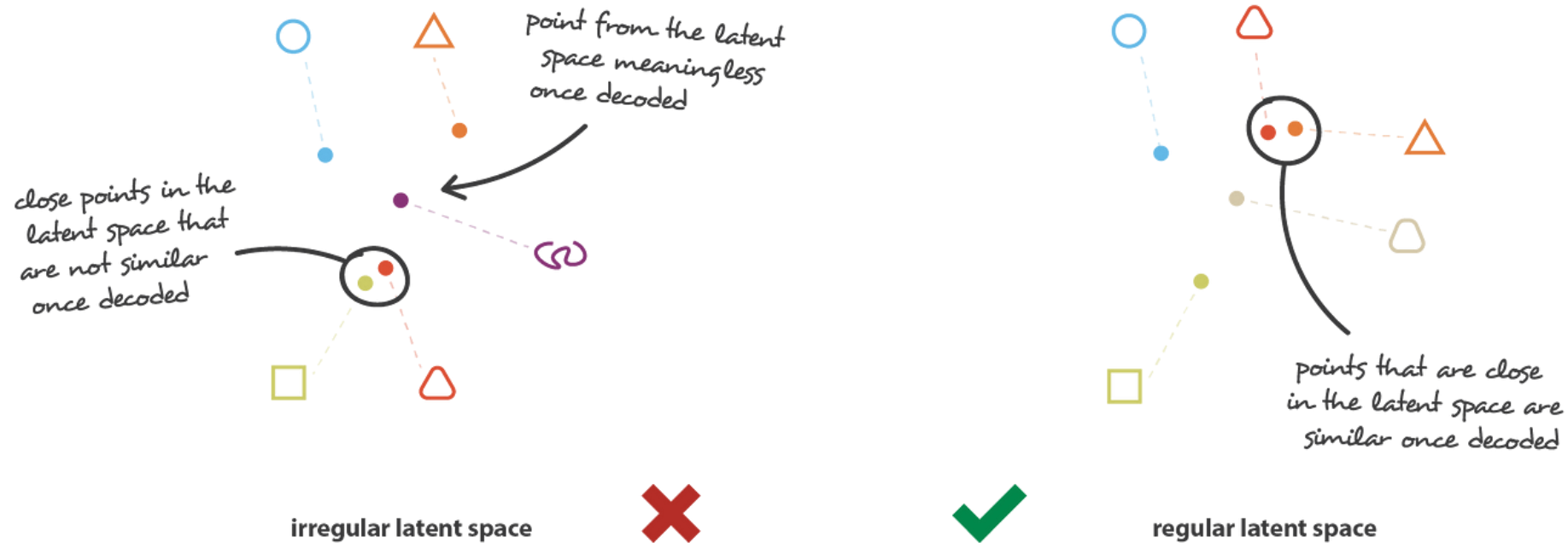


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Can AEs learn such latent spaces that are good for reconstruction + generation? **Yes, VAEs [7,8]!**

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$$\begin{aligned} p_{\theta}(X) &= \int_{\mathcal{Z}} p_{\theta}(X, Z) dZ \\ &= \int_{\mathcal{Z}} p_{\theta}(X|Z) p_{\theta}(Z) dZ \end{aligned}$$

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Intractable Integration!

Evidence Lower Bound (ELBO)

Variational Approximation

$$\begin{aligned}\log p_{\theta}(X) &= \log \left(\frac{p_{\theta}(X, Z)}{p_{\theta}(Z|X)} \right) \\ &= \log \left(\frac{p_{\theta}(X, Z) q_{\phi}(Z|X)}{q_{\phi}(Z|X) p_{\theta}(Z|X)} \right)\end{aligned}$$

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Integrating from both sides:

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Evidence Lower Bound (ELBO) Kullback-Leibler (KL) Divergence

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Integrating from both sides:

Why is it a lower bound?

$$\begin{aligned}\log p_{\theta}(X) &= \int q_{\phi}(Z|X) \log p_{\theta}(X) dZ \\ &= \int q_{\phi}(Z|X) \log \left(\frac{p_{\theta}(X, Z) q_{\phi}(Z|X)}{q_{\phi}(Z|X) p_{\theta}(Z|X)} \right) dZ \\ &= \int q_{\phi}(Z|X) \log \left(\frac{p_{\theta}(X, Z)}{q_{\phi}(Z|X)} \right) dZ + \int q_{\phi}(Z|X) \log \left(\frac{q_{\phi}(Z|X)}{p_{\theta}(Z|X)} \right) dZ \\ &= \underbrace{\mathbb{E}_{q_{\phi}(Z|X)} \left[\log \left(\frac{p_{\theta}(X, Z)}{q_{\phi}(Z|X)} \right) \right]}_{\text{Evidence Lower Bound (ELBO)}} + \underbrace{\text{KL} (q_{\phi}(Z|X) || p_{\theta}(Z|X))}_{\text{Kullback-Leibler (KL) Divergence}}\end{aligned}$$

Evidence Lower Bound (ELBO) Kullback-Leibler (KL) Divergence

Evidence Lower Bound (ELBO)

Variational Approximation

$$\begin{aligned}\log p_{\theta}(X) &= \log \left(\frac{p_{\theta}(X, Z)}{p_{\theta}(Z|X)} \right) \\ &= \log \left(\frac{p_{\theta}(X, Z) q_{\phi}(Z|X)}{q_{\phi}(Z|X) p_{\theta}(Z|X)} \right)\end{aligned}$$

Integrating from both sides:

Why is it a lower bound? **KL is nonnegative!**

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Evidence Lower Bound (ELBO)

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Why is it called variational approximation?

Evidence Lower Bound (ELBO) Kullback-Leibler (KL) Divergence

Evidence Lower Bound (ELBO)

Variational Approximation

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Why is it a lower bound? **KL is nonnegative!**

Why is it called variational approximation?
We choose one distribution (function) from a family to approximate the target!

Evidence Lower Bound (ELBO) Kullback-Leibler (KL) Divergence

Evidence Lower Bound (ELBO)

Since true posterior $p_{\theta}(Z|X)$ is often unknown, KL term is intractable

Evidence Lower Bound (ELBO)

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ELBO:

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Evidence Lower Bound (ELBO)

Since true posterior $p_\theta(Z|X)$ is often unknown, KL term is intractable

ELBO:

$$\begin{aligned}\mathbb{E}_{q_\phi(Z|X)} \left[\log \left(\frac{p_\theta(X, Z)}{q_\phi(Z|X)} \right) \right] &= \mathbb{E}_{q_\phi(Z|X)} \left[\log \left(\frac{p_\theta(X|Z)p_\theta(Z)}{q_\phi(Z|X)} \right) \right] \\ &= \mathbb{E}_{q_\phi(Z|X)} [\log (p_\theta(X|Z))] + \mathbb{E}_{q_\phi(Z|X)} \left[\log \left(\frac{p_\theta(Z)}{q_\phi(Z|X)} \right) \right] \\ &= \underbrace{-\mathbb{E}_{q_\phi(Z|X)} [-\log (p_\theta(X|Z))]}_{\text{Reconstruction Error/Loss}} - \underbrace{\text{KL} (q_\phi(Z|X) \| p_\theta(Z))}_{\text{Regularizer}}\end{aligned}$$

Evidence Lower Bound (ELBO)

Since true posterior $p_\theta(Z|X)$ is often unknown, KL term is intractable

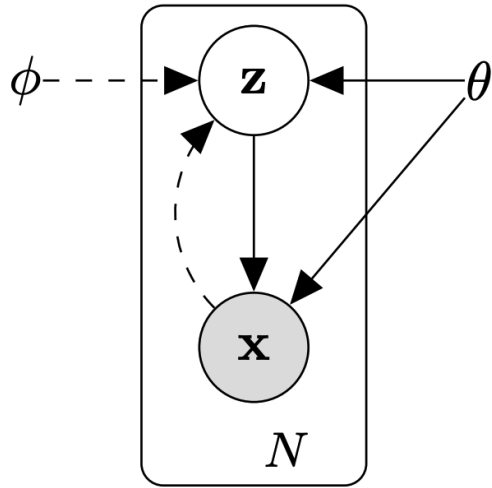
ELBO:

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Outline

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 - Motivation & Overview
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 - Amortized Inference
 - Reparameterization Trick

Variational Autoencoders

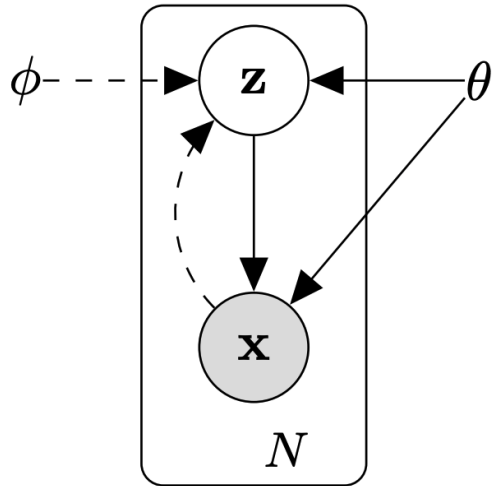


Encoder: $q_{\phi}(Z|X)$

Decoder: $p_{\theta}(X|Z)$

Prior: $p_{\theta}(Z)$

Variational Autoencoders



Since we typically use continuous latent variable Z , Gaussian distribution is a natural choice for the encoder:

$$q_{\phi}(Z|X) = \mathcal{N}(Z|\mu, \sigma^2 I)$$

$$\mu = \text{EncoderNetwork}_{\phi}(X)$$

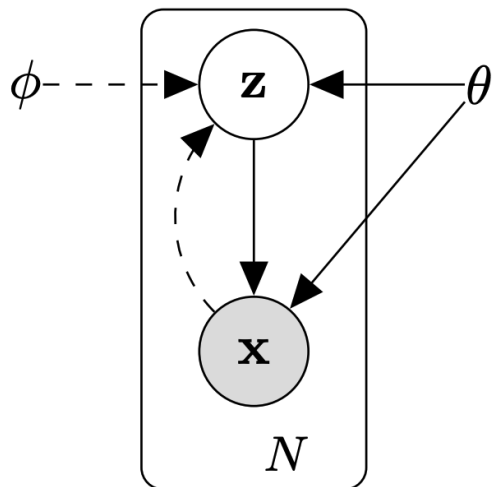
$$\log \sigma^2 = \text{EncoderNetwork}_{\phi}(X)$$

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Similarly, Gaussian distribution is often adopted for the decoder:

$$p_{\theta}(X|Z) = \mathcal{N}(X|\tilde{\mu}, \tilde{\sigma}^2 I)$$

$$\tilde{\mu} = \text{DecoderNetwork}_{\theta}(Z)$$

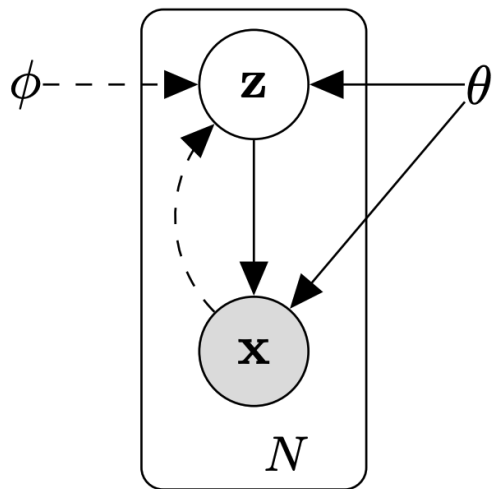
$$\log \tilde{\sigma}^2 = \text{DecoderNetwork}_{\theta}(Z)$$

Encoder: $q_{\phi}(Z|X)$

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Variational Autoencoders



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We often fix the prior as, e.g., standard Normal $p_{\theta}(Z) = \mathcal{N}(Z|\mathbf{0}, I)$

Variational Autoencoders

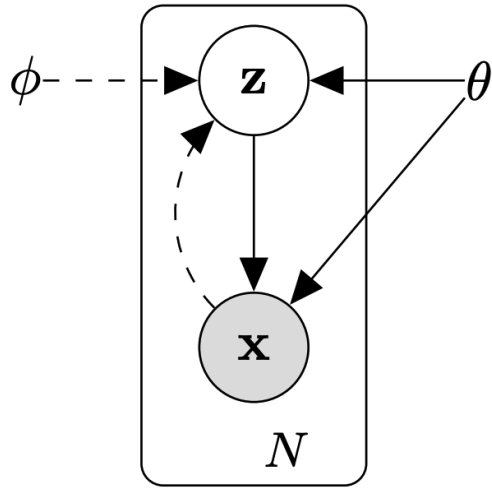
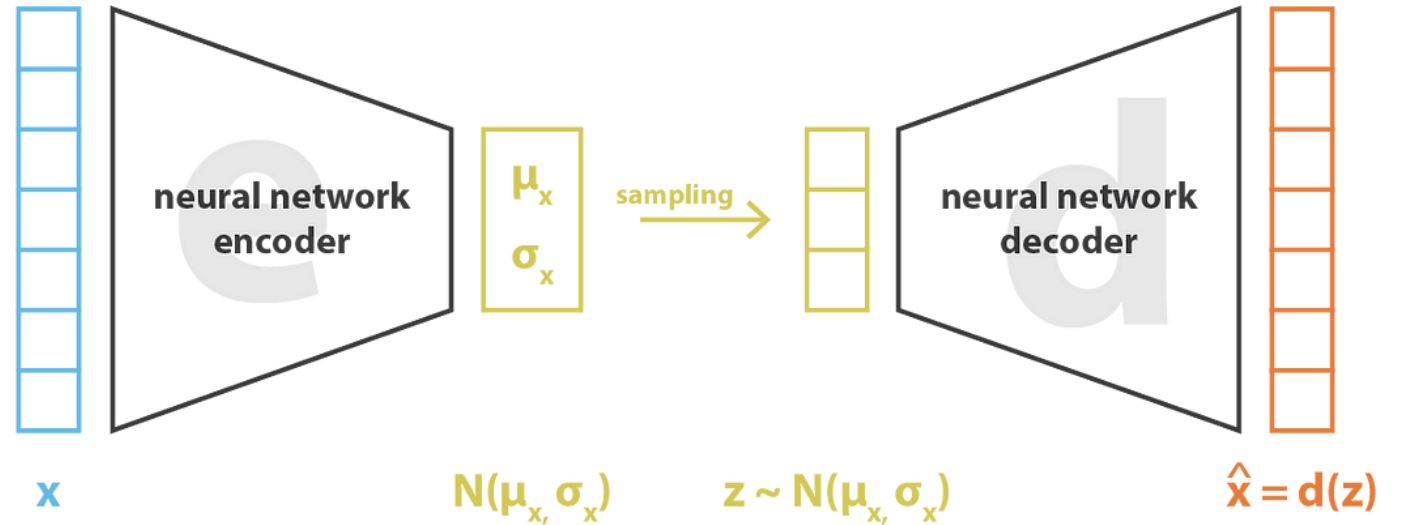


Illustration of VAEs:



Encoder: $q_{\phi}(Z|X)$

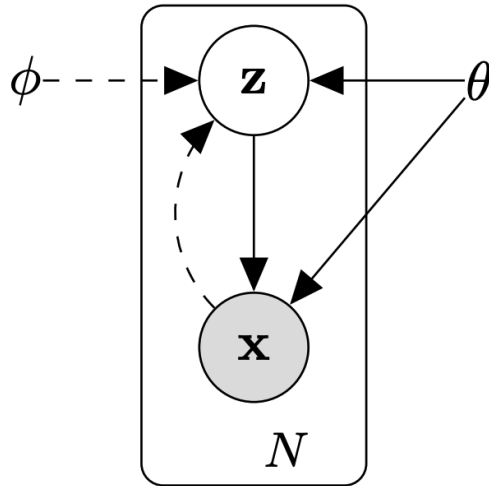
Decoder: $p_{\theta}(X|Z)$

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Outline

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 - Reparameterization Trick

Amortized Variational Inference



Since we typically use continuous latent variable Z , Gaussian distribution is a natural choice for the encoder:

$$q_\phi(Z|X) = \mathcal{N}(Z|\mu, \sigma^2 I)$$

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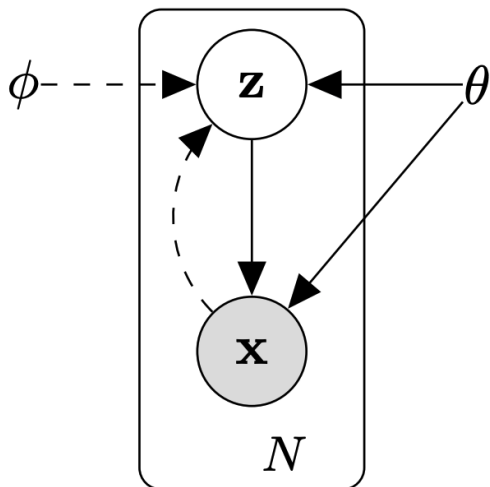
Encoder is **amortized**: every X shares the same set of parameters ϕ

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Amortized Variational Inference



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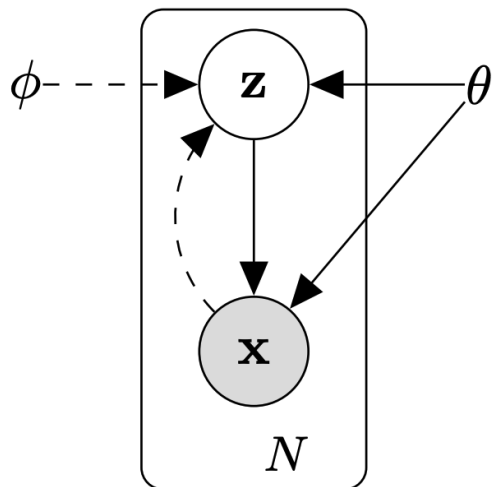
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We thus only need to optimize ELBO over one set of parameters ϕ , whereas in traditional variational inference (VI) one needs to find the optimal variational distribution per X

Amortized Variational Inference



Since we typically use continuous latent variable Z , Gaussian distribution is a natural choice for the encoder:

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We thus only need to optimize ELBO over one set of parameters ϕ , whereas in traditional variational inference (VI) one needs to find the optimal variational distribution per X

Different X still have different encoder distributions $q_{\phi}(Z|X)$

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Reparameterization Trick

Negative ELBO: $\mathcal{L}(\phi, \theta) = \underbrace{\mathbb{E}_{q_\phi(Z|X)} [-\log(p_\theta(X|Z))]}_{\text{Reconstruction Error/Loss}} + \underbrace{\text{KL}(q_\phi(Z|X) \| p_\theta(Z))}_{\text{Regularizer}}$

We want to minimize negative ELBO w.r.t. encoder parameters ϕ and decoder parameters θ

Reparameterization Trick

Negative ELBO: $\mathcal{L}(\phi, \theta) = \underbrace{\mathbb{E}_{q_\phi(Z|X)} [-\log(p_\theta(X|Z))]}_{\text{Reconstruction Error/Loss}} + \underbrace{\text{KL}(q_\phi(Z|X) \| p_\theta(Z))}_{\text{Regularizer}}$

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The expectation in reconstruction loss is intractable and often approximated by Monte Carlo estimation

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We will use *reparameterization trick* to equivalently rewrite the expectation in reconstruction loss so that the Monte Carlo gradient w.r.t. ϕ has a lower variance.

Reparameterization Trick

For any function f , we have

$$\begin{aligned}\mathbb{E}_{\mathcal{N}(Z|\mu, \sigma^2 I)} [f(Z)] &= \int \frac{1}{\sqrt{(2\pi)^m \prod_i \sigma_i}} \exp\left(-\frac{1}{2} \left\| \frac{Z - \mu}{\sigma} \right\|^2\right) f(Z) dZ \\ &= \int \frac{1}{\sqrt{(2\pi)^m \prod_i \sigma_i}} \exp\left(-\frac{1}{2} \left\| \frac{\mu + \sigma\epsilon - \mu}{\sigma} \right\|^2\right) f(\mu + \sigma\epsilon) d(\mu + \sigma\epsilon) \\ &= \int \frac{1}{\sqrt{(2\pi)^m}} \exp\left(-\frac{1}{2} \|\epsilon\|^2\right) f(\mu + \sigma\epsilon) d\epsilon \\ &= \mathbb{E}_{\mathcal{N}(\epsilon|0, I)} [f(\mu + \sigma\epsilon)]\end{aligned}$$

Change of Variable

Reparameterization Trick

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Change of Variable

Therefore,

$$\begin{aligned}\mathcal{L}(\phi, \theta) &= \mathbb{E}_{q_\phi(Z|X)} [-\log(p_\theta(X|Z))] + \text{KL}(q_\phi(Z|X) \| p_\theta(Z)) \\ &= \mathbb{E}_{\mathcal{N}(\epsilon|0, I)} [-\log(p_\theta(X|\mu_\phi(X) + \sigma_\phi(X)\epsilon))] + \text{KL}(q_\phi(Z|X) \| p_\theta(Z))\end{aligned}$$

Reparameterization Trick

In original VAE,

$$q_{\phi}(Z|X) = \mathcal{N}(Z|\mu_{\phi}(X), \sigma_{\phi}(X)^2 I)$$

$$p_{\theta}(Z) = \mathcal{N}(X|0, I)$$

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In original VAE,

$$q_\phi(Z|X) = \mathcal{N}(Z|\mu_\phi(X), \sigma_\phi(X)^2 I)$$
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Using Gaussian integrals, we have

$$\text{KL}(q_\phi(Z|X)||p_\theta(Z)) = \frac{1}{2} (\mu_\phi(X)^\top \mu_\phi(X) + \sigma_\phi(X)^\top \sigma_\phi(X)) - \frac{1}{2} \sum_{i=1}^m \log \sigma_i^2 - \frac{m}{2}$$

where

$$\sigma_\phi(X) = [\sigma_1, \sigma_2, \dots, \sigma_m]^\top$$

Reparameterization Trick

Therefore, in original VAE, we have

$$\begin{aligned}\mathcal{L}(\phi, \theta) = & \mathbb{E}_{\mathcal{N}(\epsilon|0, I)} [-\log (p_{\theta}(X|\mu_{\phi}(X) + \sigma_{\phi}(X)\epsilon))] \\ & + \frac{1}{2} (\mu_{\phi}(X)^{\top} \mu_{\phi}(X) + \sigma_{\phi}(X)^{\top} \sigma_{\phi}(X)) - \frac{1}{2} \sum_{i=1}^m \log \sigma_i^2 - \frac{m}{2}\end{aligned}$$

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We only need *reparameterization trick* and *Monte Carlo estimation* in the first term

$$\begin{aligned}\mathcal{L}(\phi, \theta) \approx & - \sum_{i=1, \epsilon_i \sim \mathcal{N}(\epsilon|0,I)}^N \log(p_{\theta}(X|\mu_{\phi}(X) + \sigma_{\phi}(X)\epsilon_i)) \\ & + \frac{1}{2} (\mu_{\phi}(X)^{\top} \mu_{\phi}(X) + \sigma_{\phi}(X)^{\top} \sigma_{\phi}(X)) - \frac{1}{2} \sum_{i=1}^m \log \sigma_i^2 - \frac{m}{2}\end{aligned}$$

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Therefore, in original VAE, we have

$$\begin{aligned}\mathcal{L}(\phi, \theta) = & \mathbb{E}_{\mathcal{N}(\epsilon|0,I)} [-\log(p_{\theta}(X|\mu_{\phi}(X) + \sigma_{\phi}(X)\epsilon))] \\ & + \frac{1}{2} (\mu_{\phi}(X)^{\top} \mu_{\phi}(X) + \sigma_{\phi}(X)^{\top} \sigma_{\phi}(X)) - \frac{1}{2} \sum_{i=1}^m \log \sigma_i^2 - \frac{m}{2}\end{aligned}$$

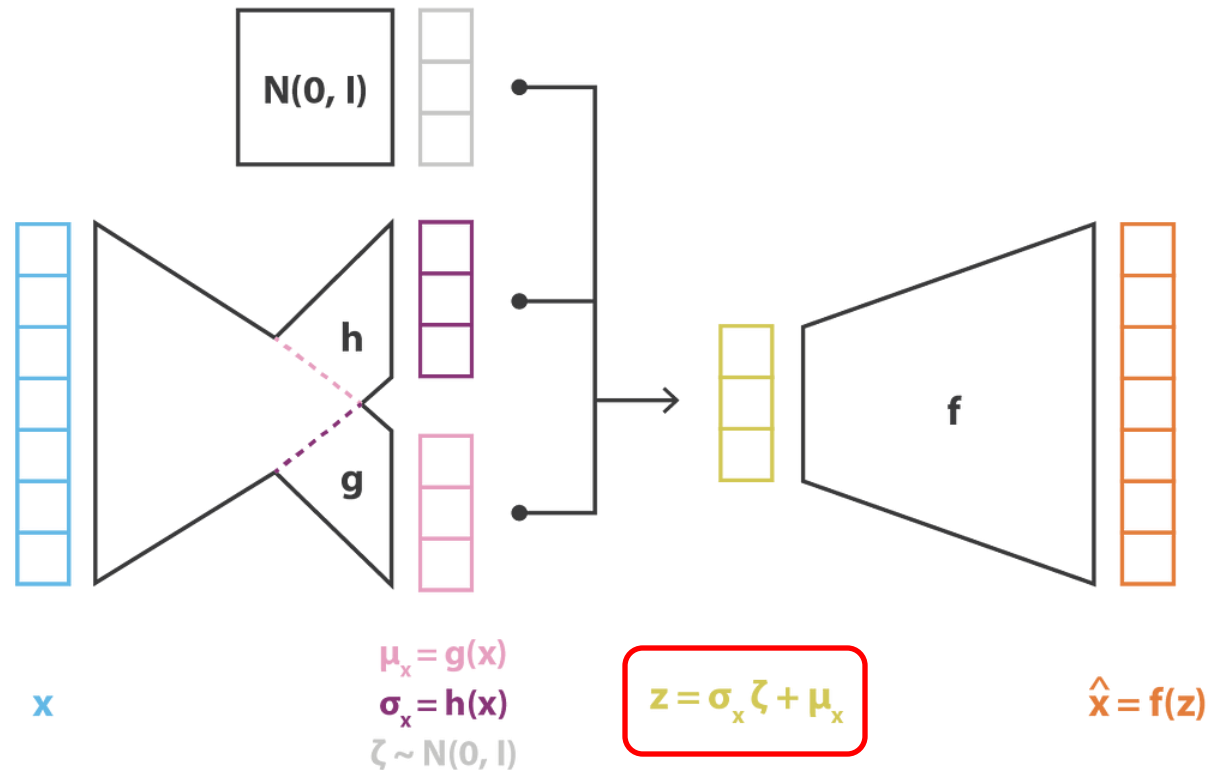
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$$\begin{aligned}\mathcal{L}(\phi, \theta) \approx & - \sum_{i=1, \epsilon_i \sim \mathcal{N}(\epsilon|0,I)}^N \log(p_{\theta}(X|\mu_{\phi}(X) + \sigma_{\phi}(X)\epsilon_i)) \\ & + \frac{1}{2} (\mu_{\phi}(X)^{\top} \mu_{\phi}(X) + \sigma_{\phi}(X)^{\top} \sigma_{\phi}(X)) - \frac{1}{2} \sum_{i=1}^m \log \sigma_i^2 - \frac{m}{2}\end{aligned}$$

Now we can get the gradient directly!

Reparameterization Trick

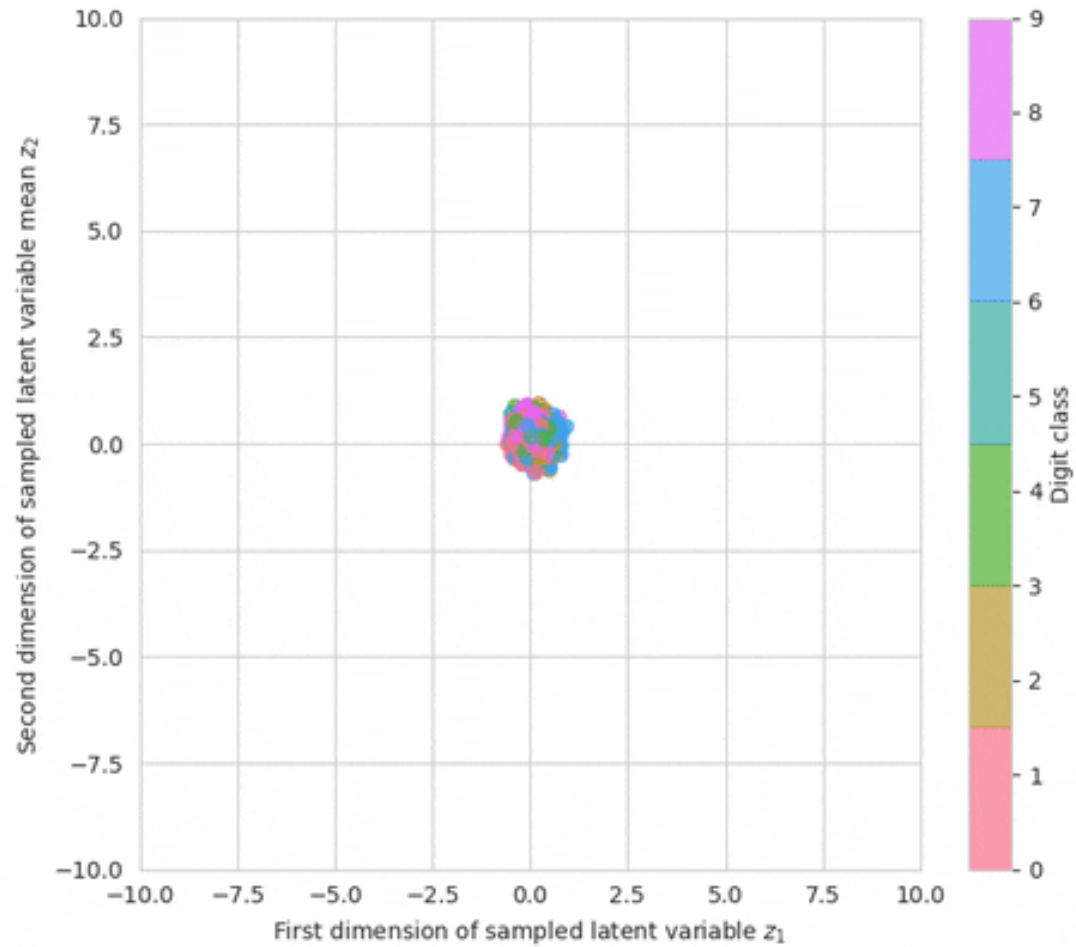
In the illustration of VAEs, the latent variable is *reparameterized* as below:



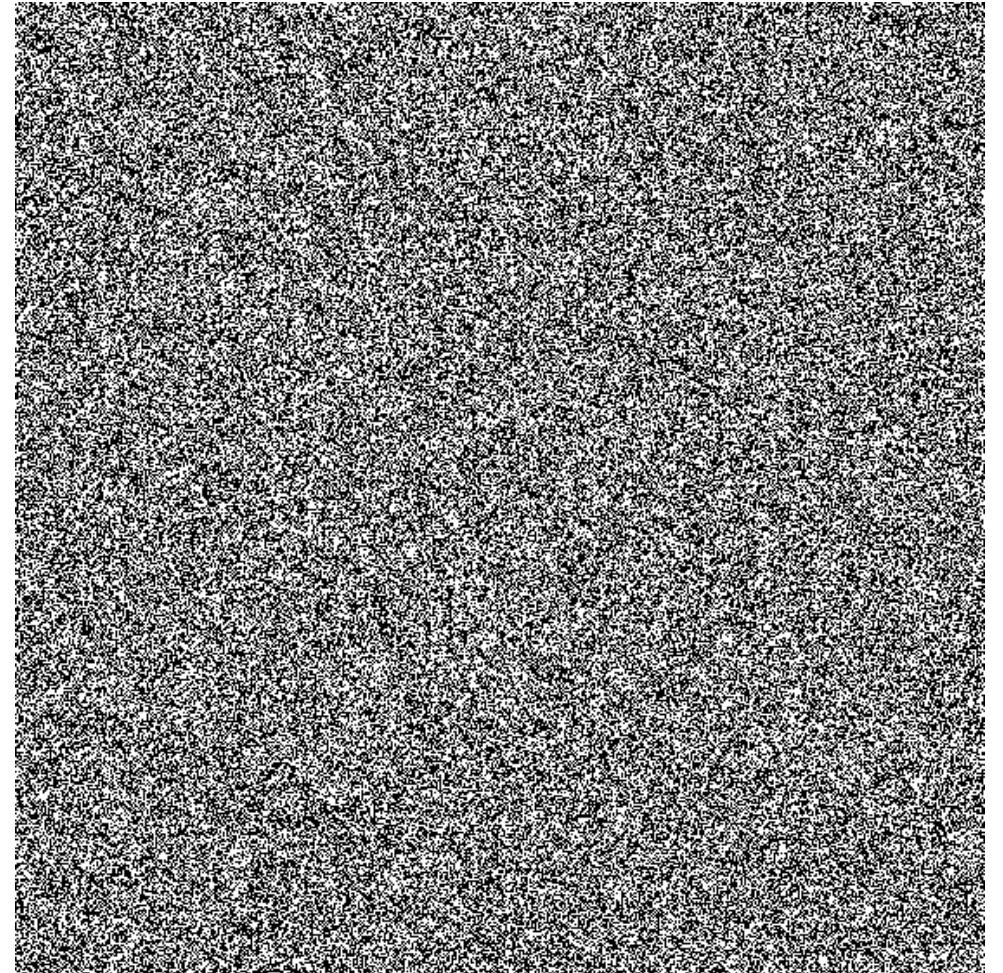
$$\text{loss} = C \|x - \hat{x}\|^2 + \text{KL}[N(\mu_x, \sigma_x), N(0, I)] = C \|x - f(z)\|^2 + \text{KL}[N(g(x), h(x)), N(0, I)]$$

VAEs on MNIST

Visualize $Z \sim q_\phi(Z|X)$ during training:



Visualize $X \sim p_\theta(X|Z)$ during training:



References

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Questions?