EECE 571F: Advanced Topics in Deep Learning

Lecture 8: Auto-Encoders & Variational Auto-Encoders

Renjie Liao

University of British Columbia

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Outline

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

Autoencoders (AEs)

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

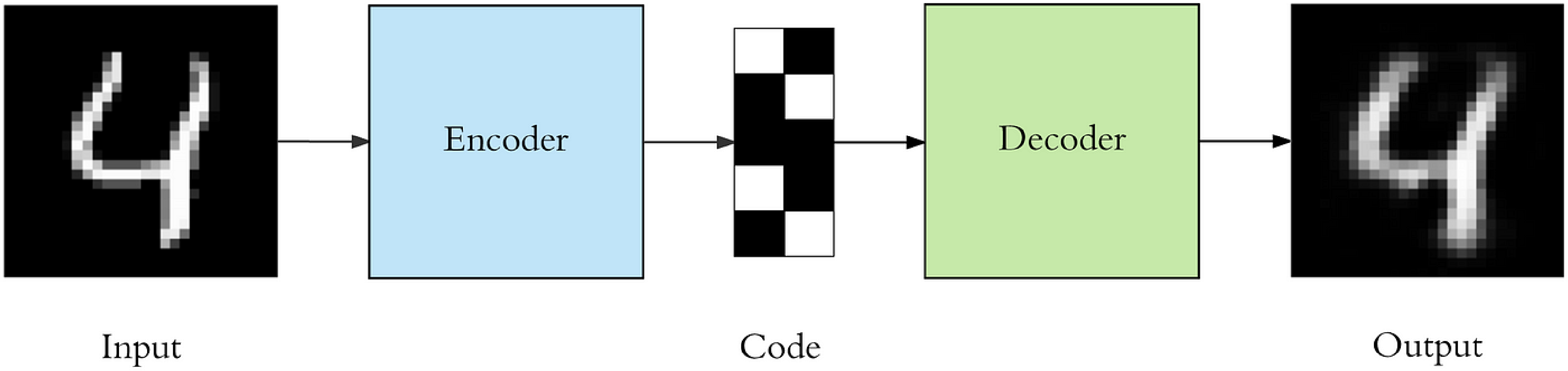

Image Credit: [1]

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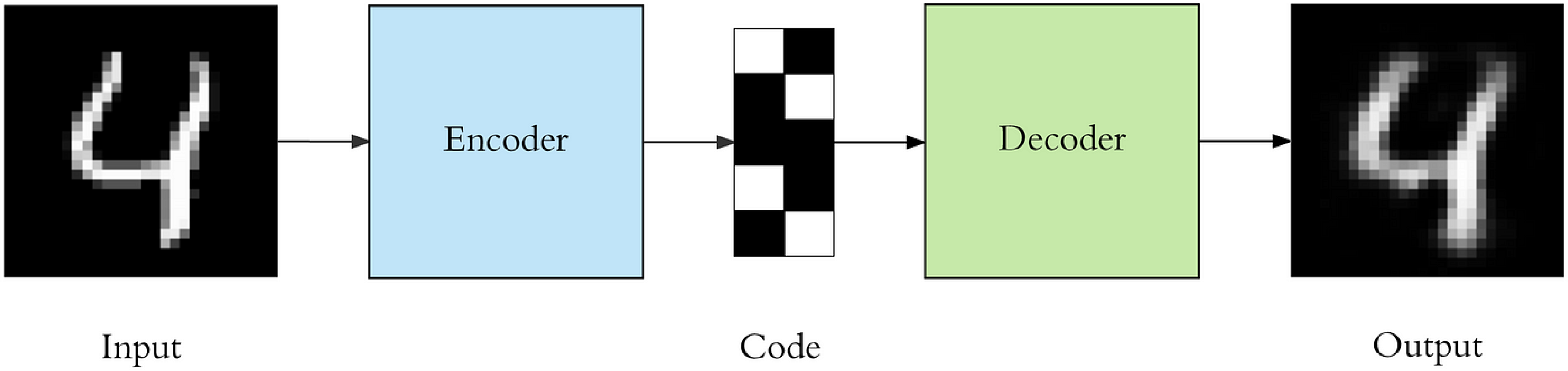
- To make it non-trivial, we need a *bottleneck* (i.e. the dimension of code being much smaller compared to the input). Why?



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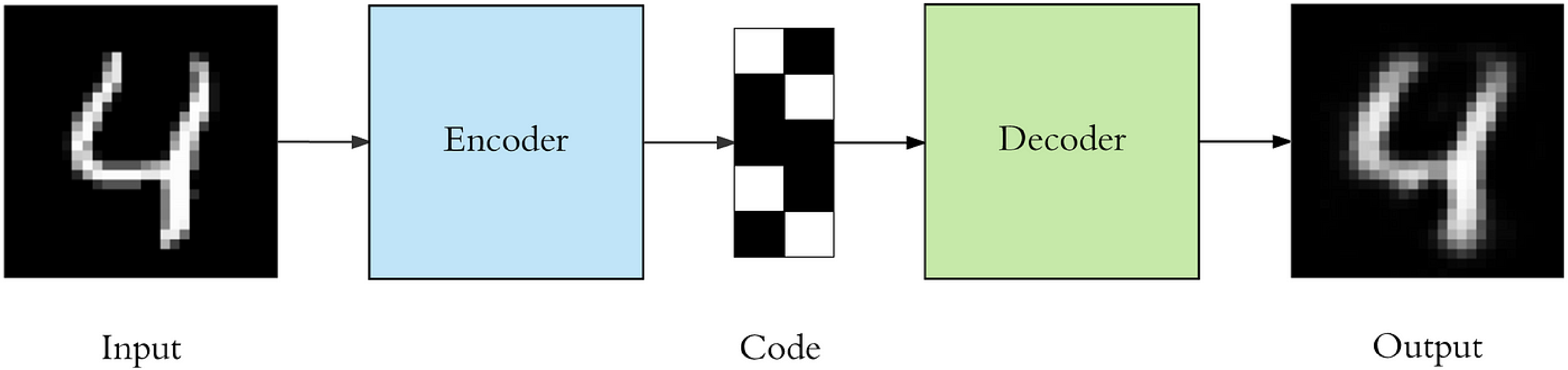

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Why should we care?

- 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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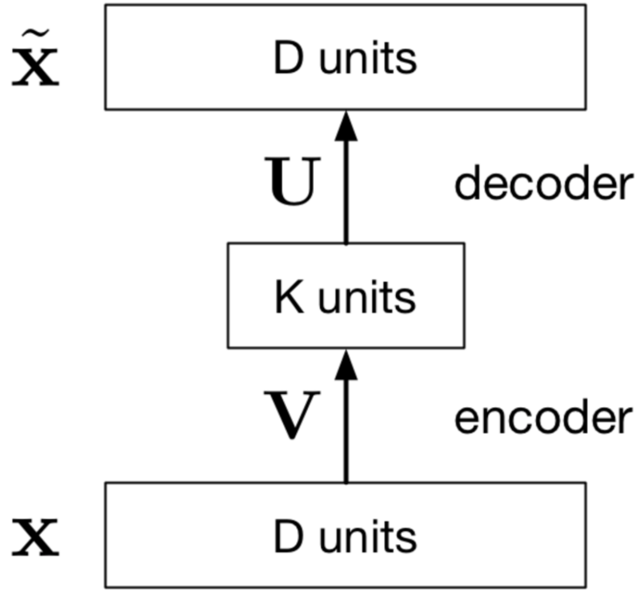
Linear Autoencoders

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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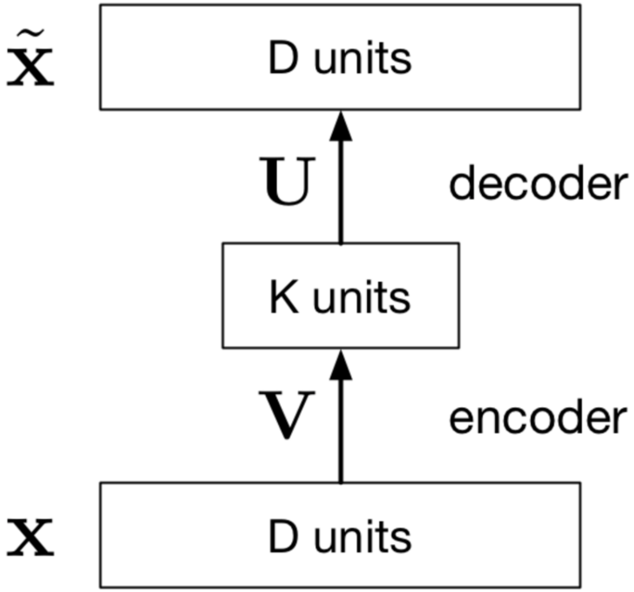
If $K \geq D$, one can choose U and V such that $UV = I$ (copying input)

Underdetermined system of equations, possibly having infinite solutions



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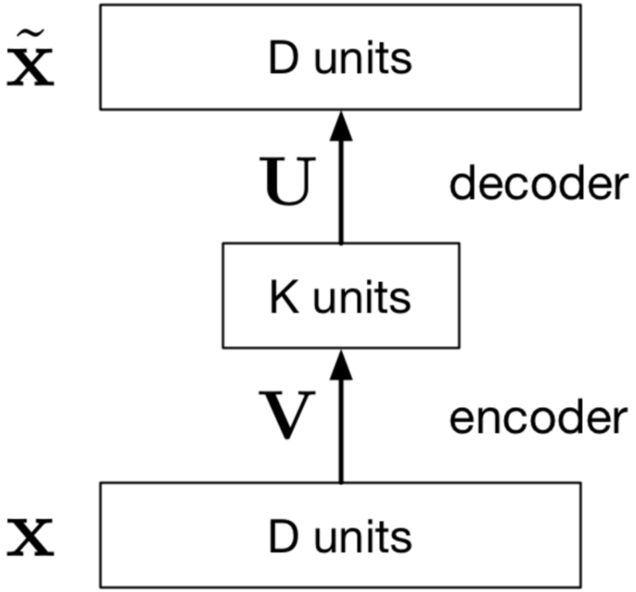
Else $K < D$, we are reducing the dimension
The reconstructed output lies in the column space of U, which is a K-dimensional subspace



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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?

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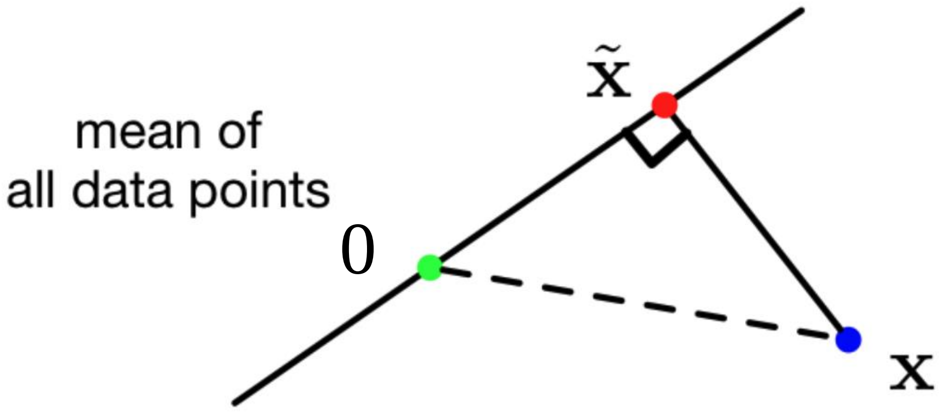
By Pythagorean Theorem, we have:

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



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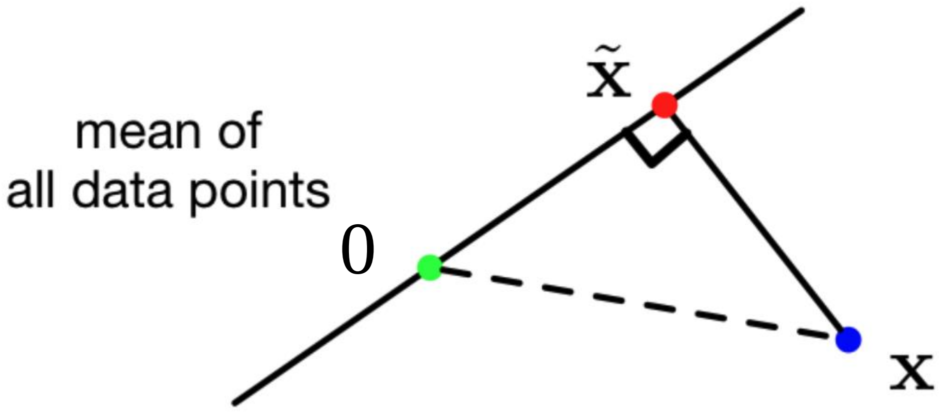

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Maximizing the projected variance is equivalent to minimizing the reconstruction error!

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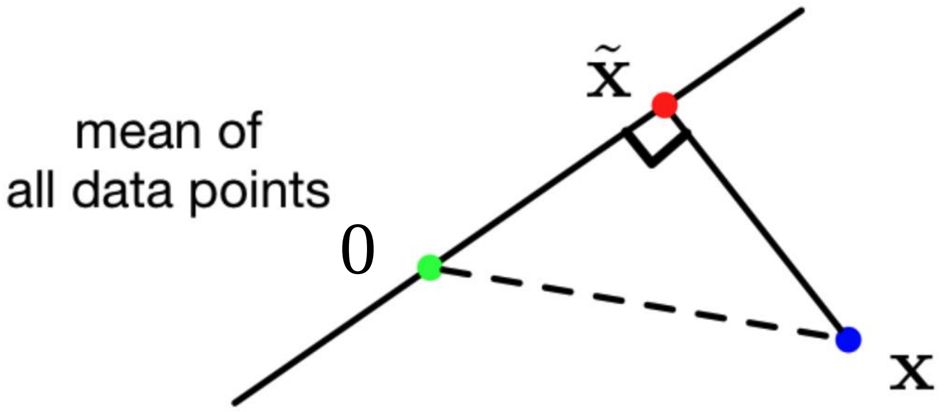

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Maximizing the projected variance is equivalent to minimizing the reconstruction error!

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

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In fact, given $\tilde{\mathbf{x}} = UV\mathbf{x}$, the minima of the reconstruction loss $\frac{1}{N}\sum_{i=1}^{N} \|\tilde{\mathbf{x}}_i - \mathbf{x}_i\|_2^2$ is not unique!

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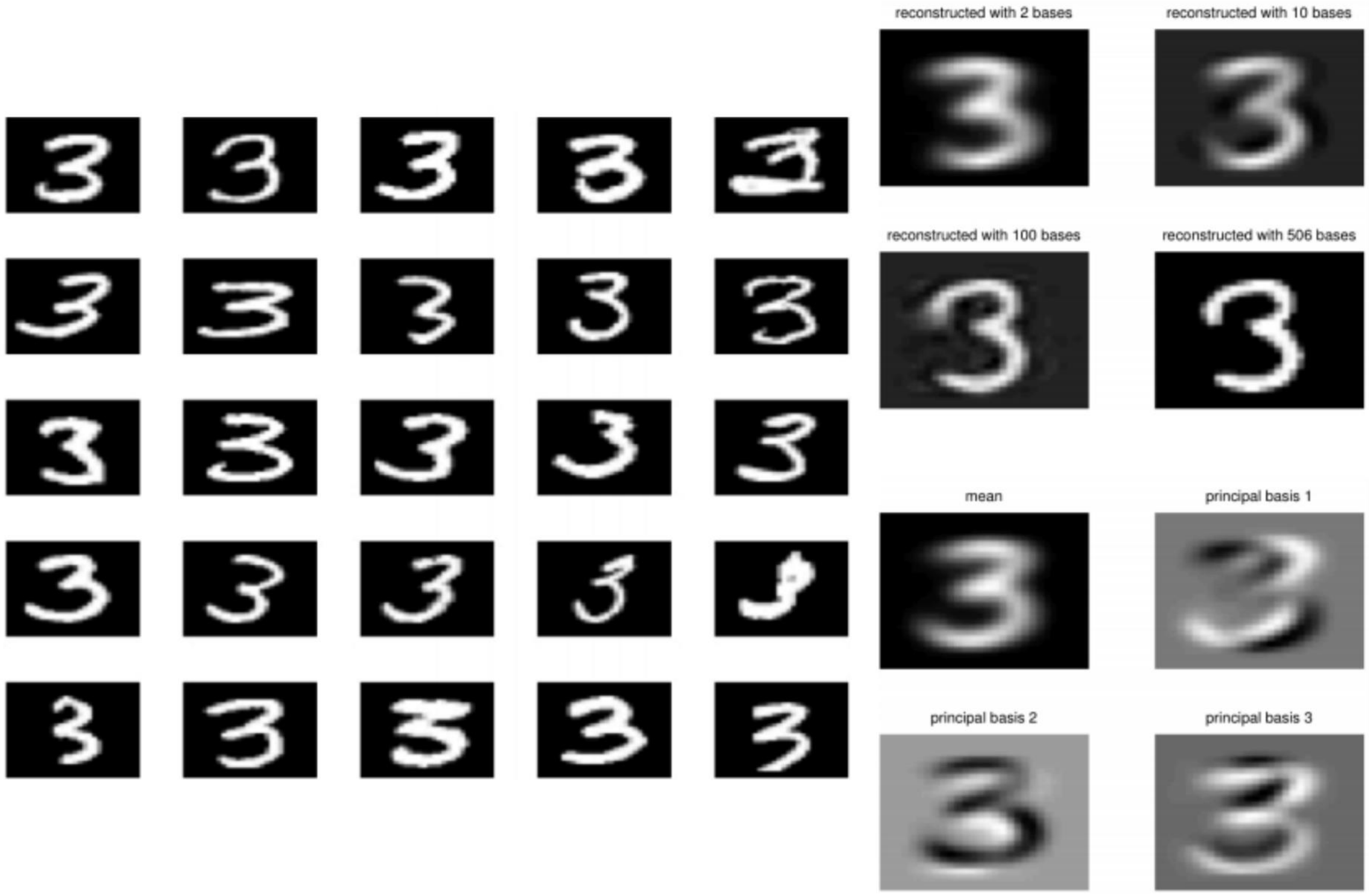
Principle components of faces ("Eigenfaces") from CBCL dataset:

Image Credit: [2]

Linear Autoencoders & Principle Component Analysis

Principle components of digits from MNIST dataset:



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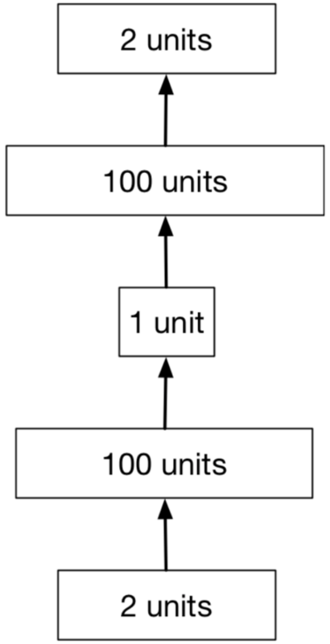
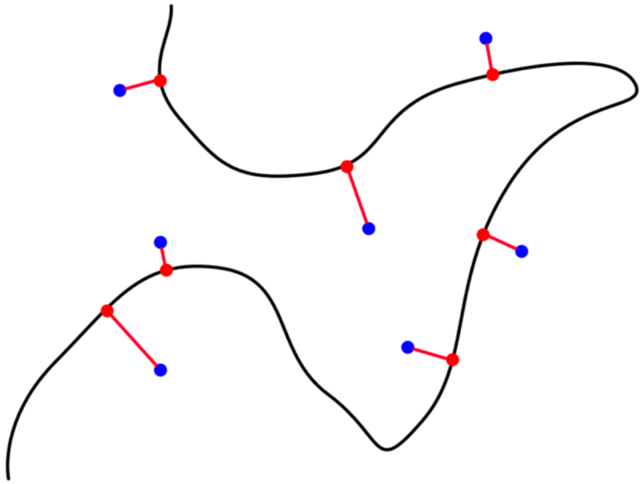
Deep Autoencoders

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

This is a kind of *nonlinear dimension reduction*





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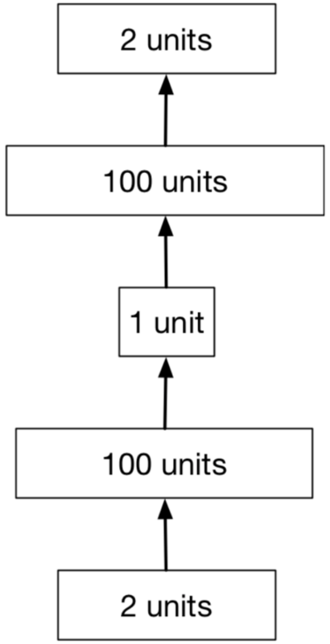

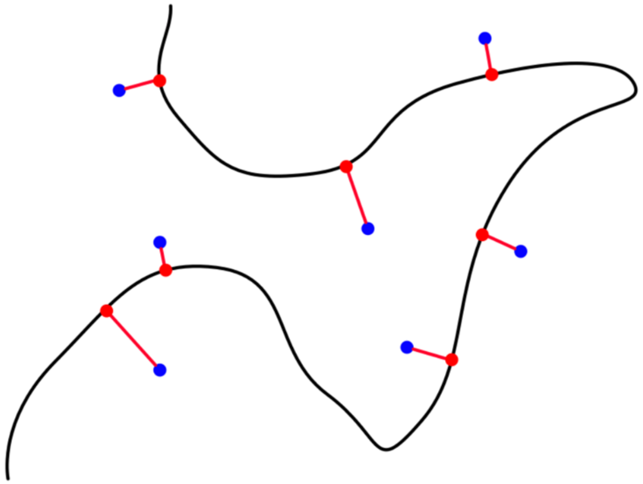

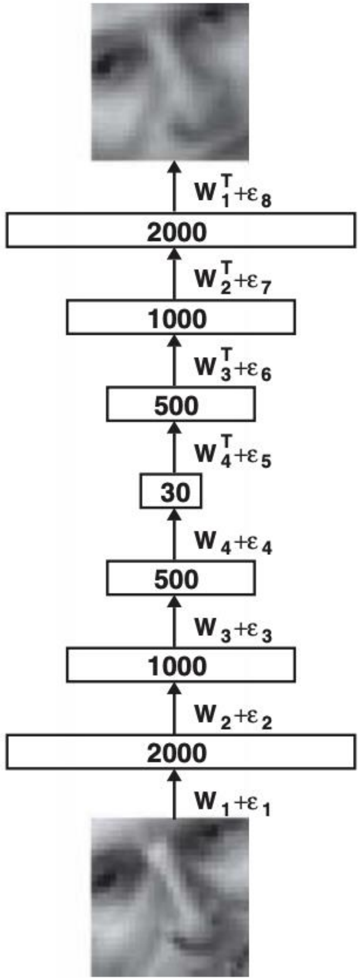

Image Credit: [2,4]

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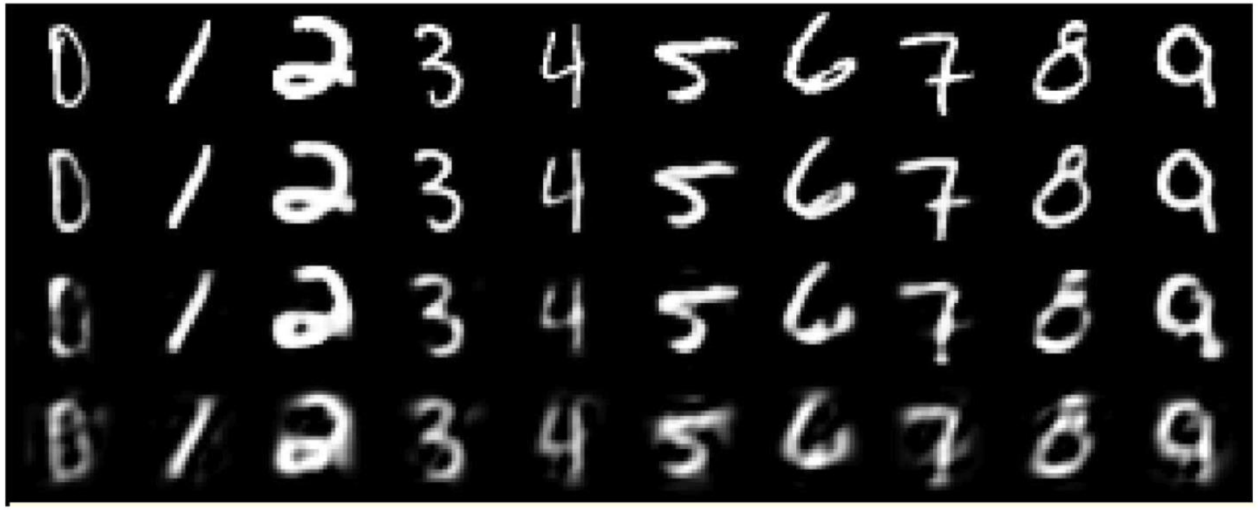
Deep autoencoders can learn more powerful codes/representations compared to linear ones (PCA)

Reconstructions with various methods on MNIST dataset:



Real data

30-d deep autoencoder

30-d logistic PCA

30-d PCA

Image Credit: [4]

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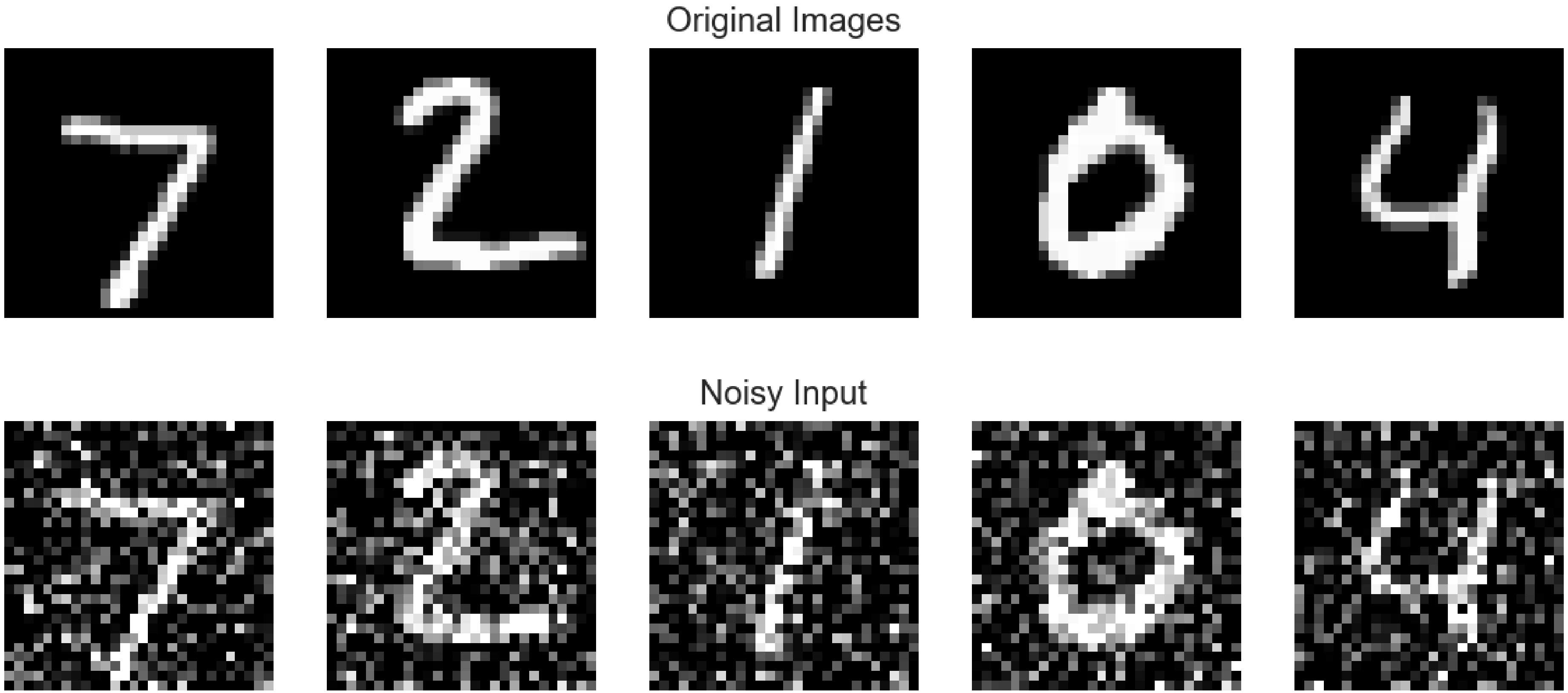

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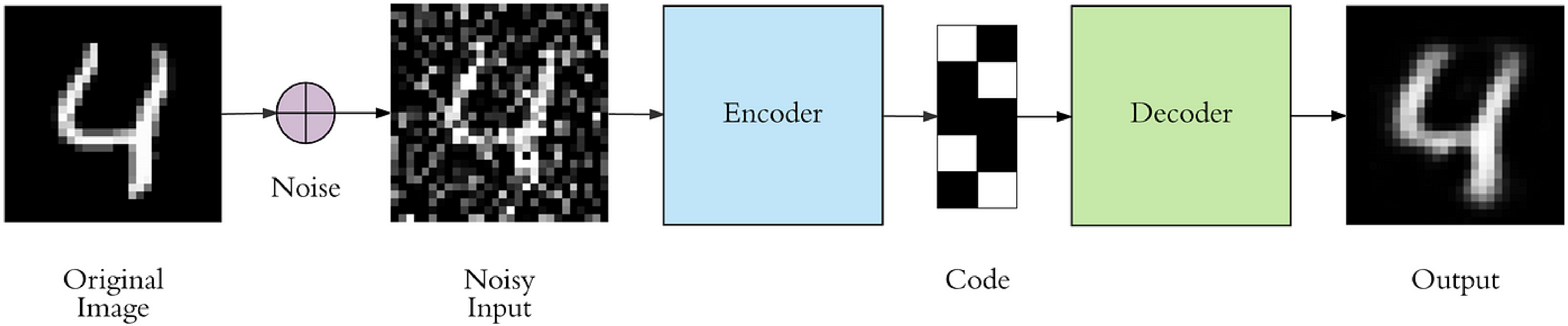
We add random noise (e.g., additive Gaussian) and force the neural network to learn useful representations so that *structures in images are preserved whereas noise is removed!*



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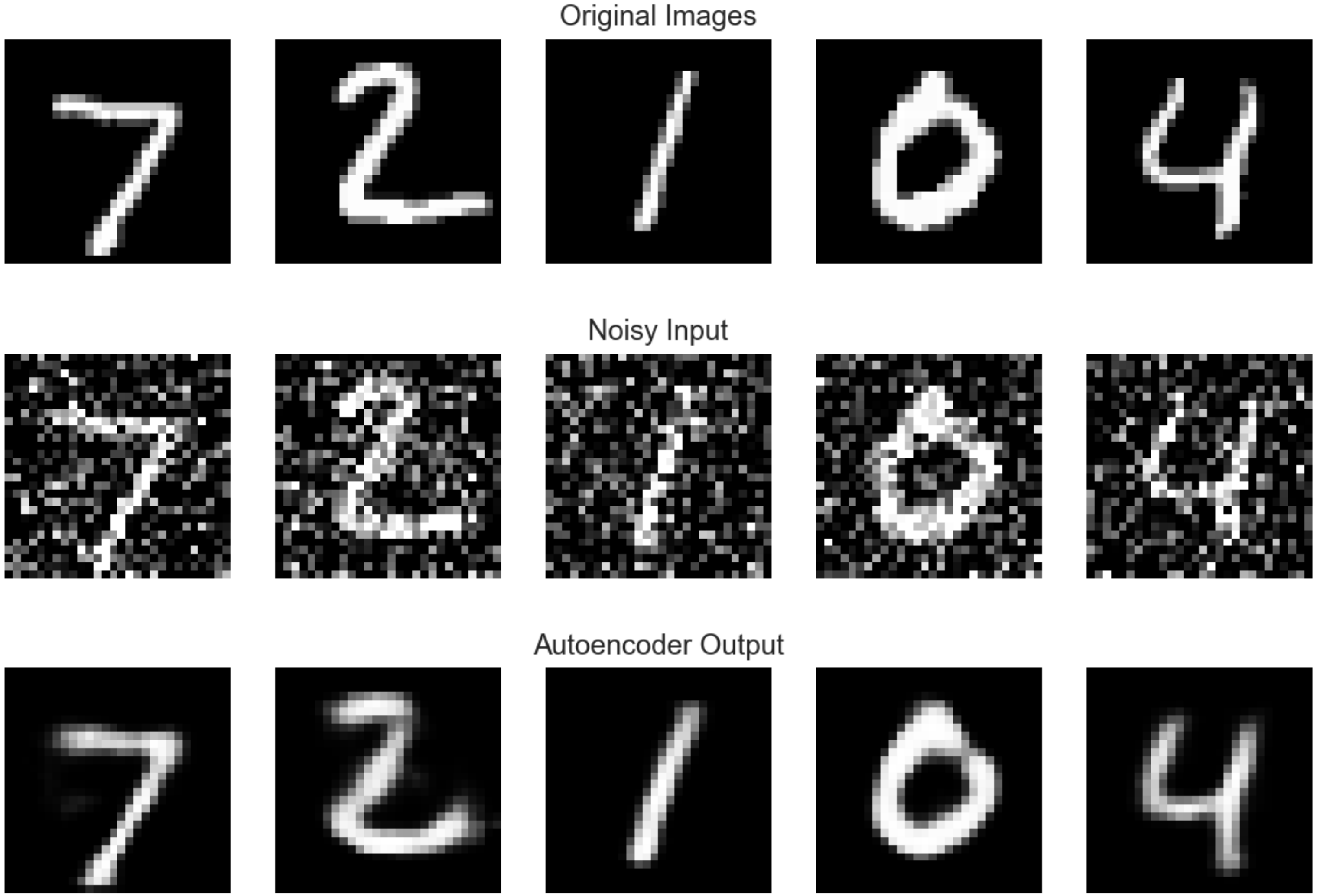
Denoising Autoencoders (DAEs)

DAEs can do a great job in denoising:



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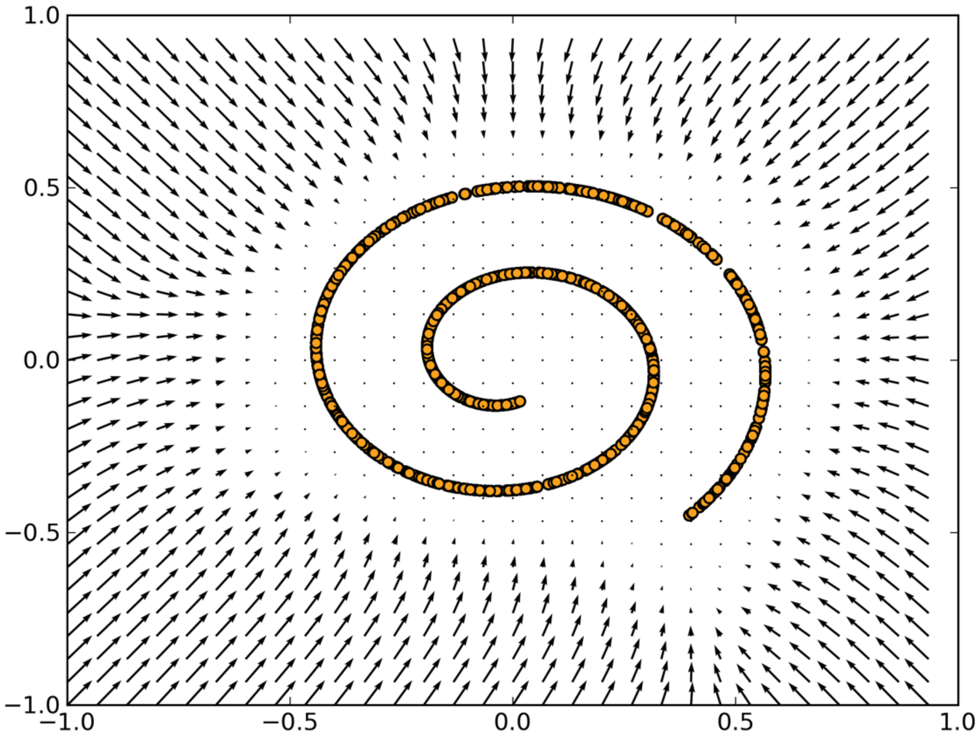
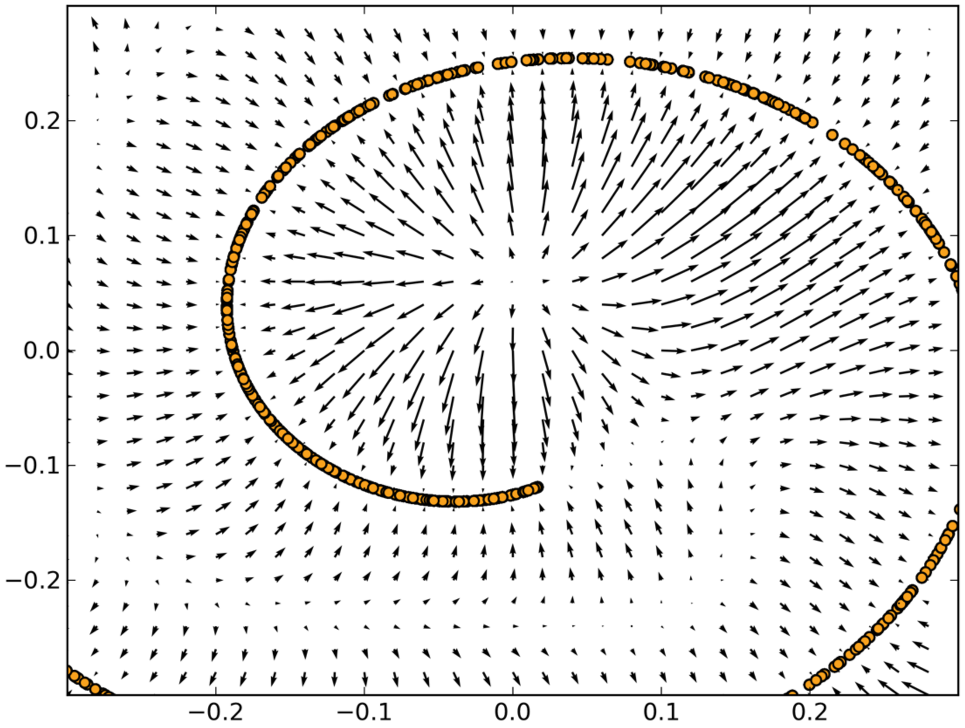
Denoising Autoencoders (DAEs)

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



zoom out



zoom in

Image Credit: [5]

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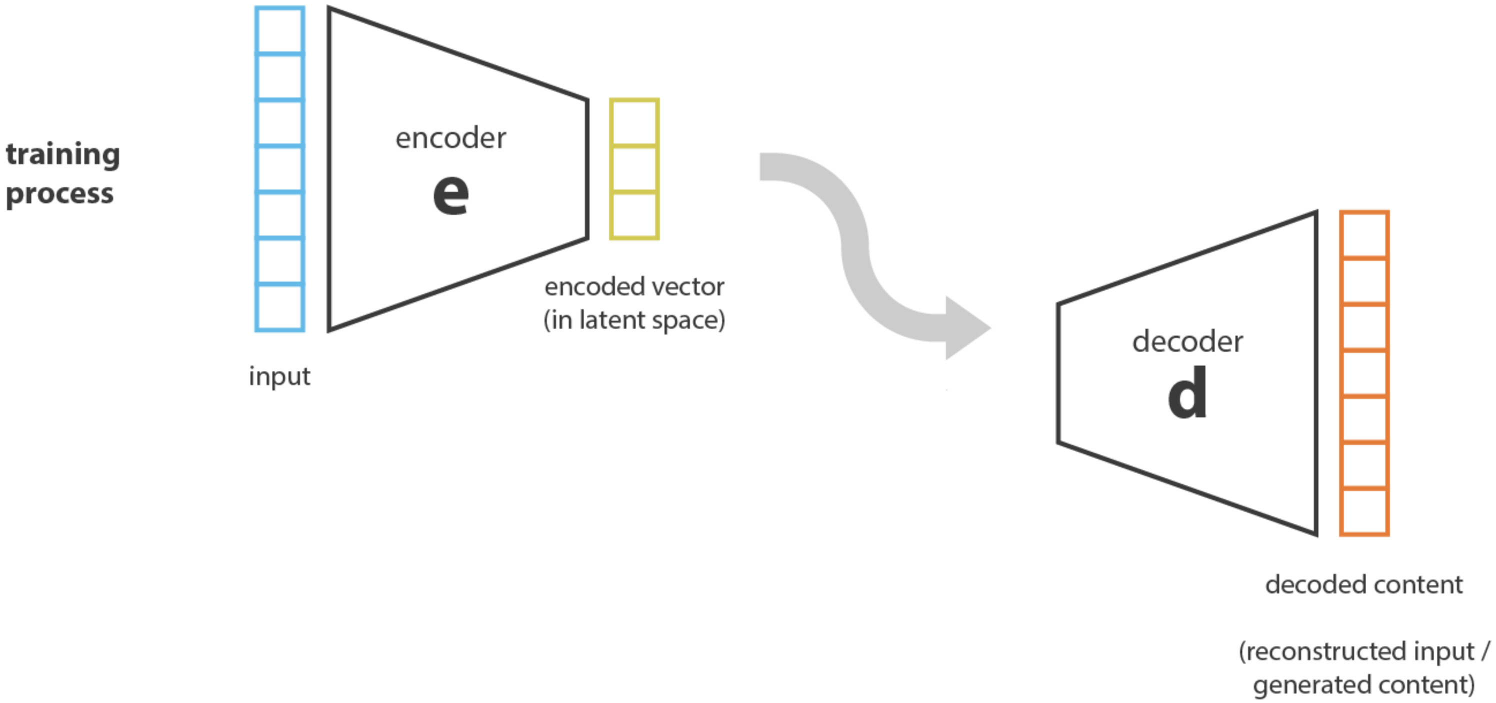

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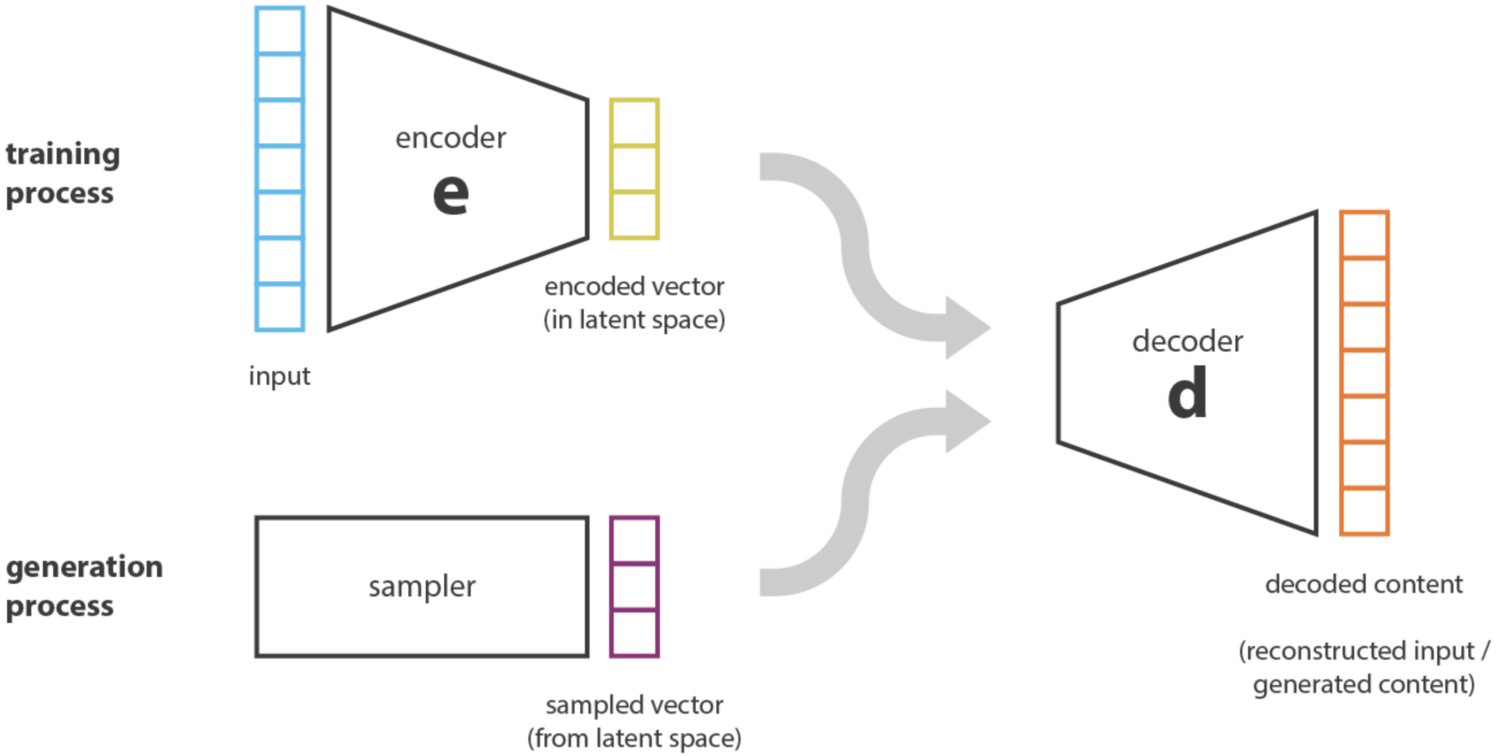

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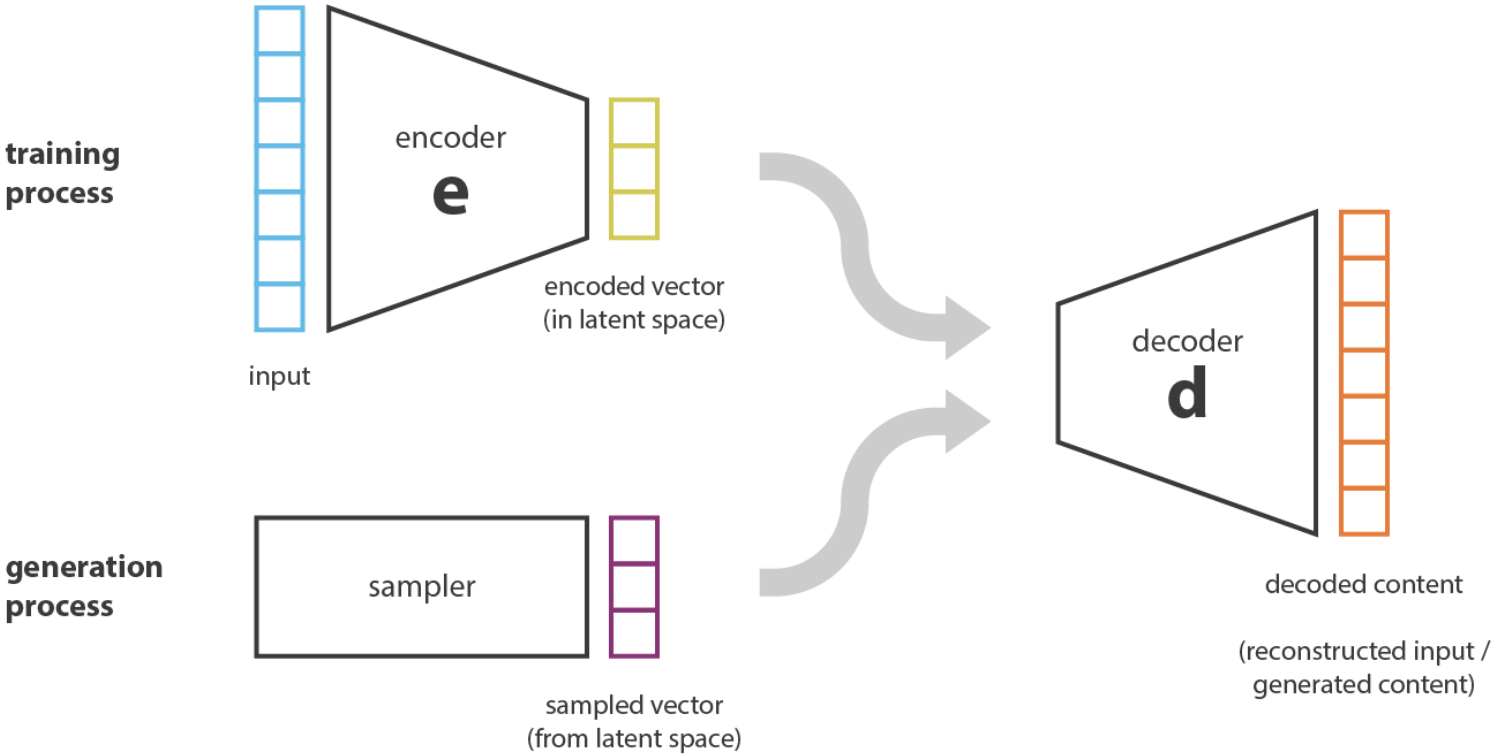

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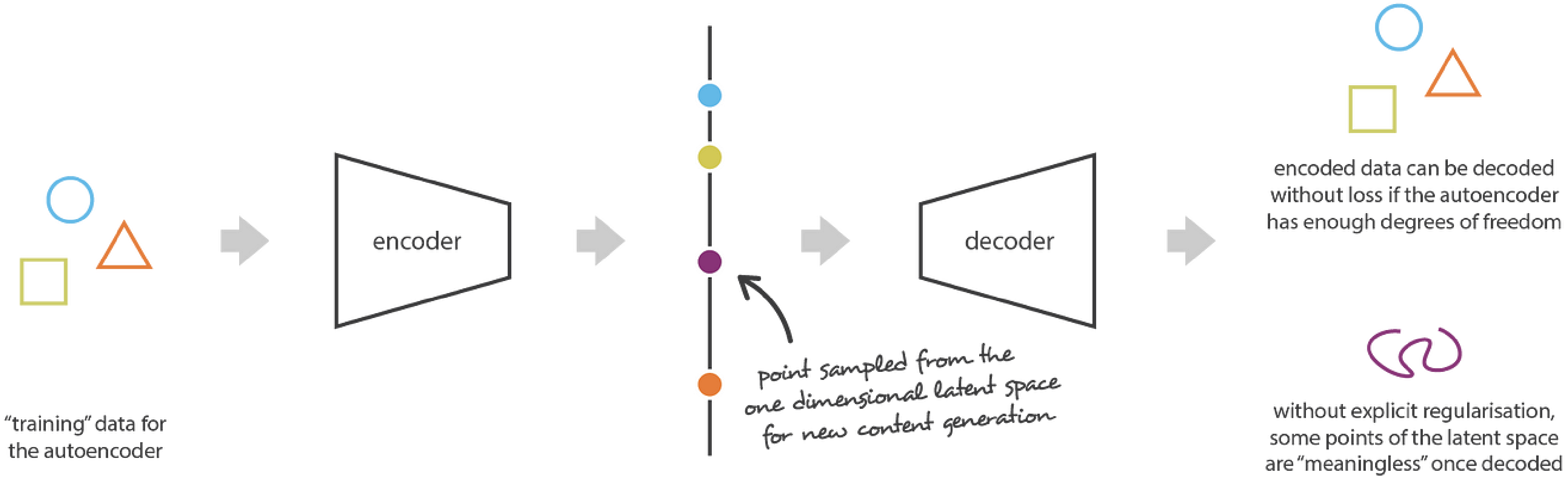
What would happen? *Sampled data could be very bad if sampled latent codes are far off the manifold!*



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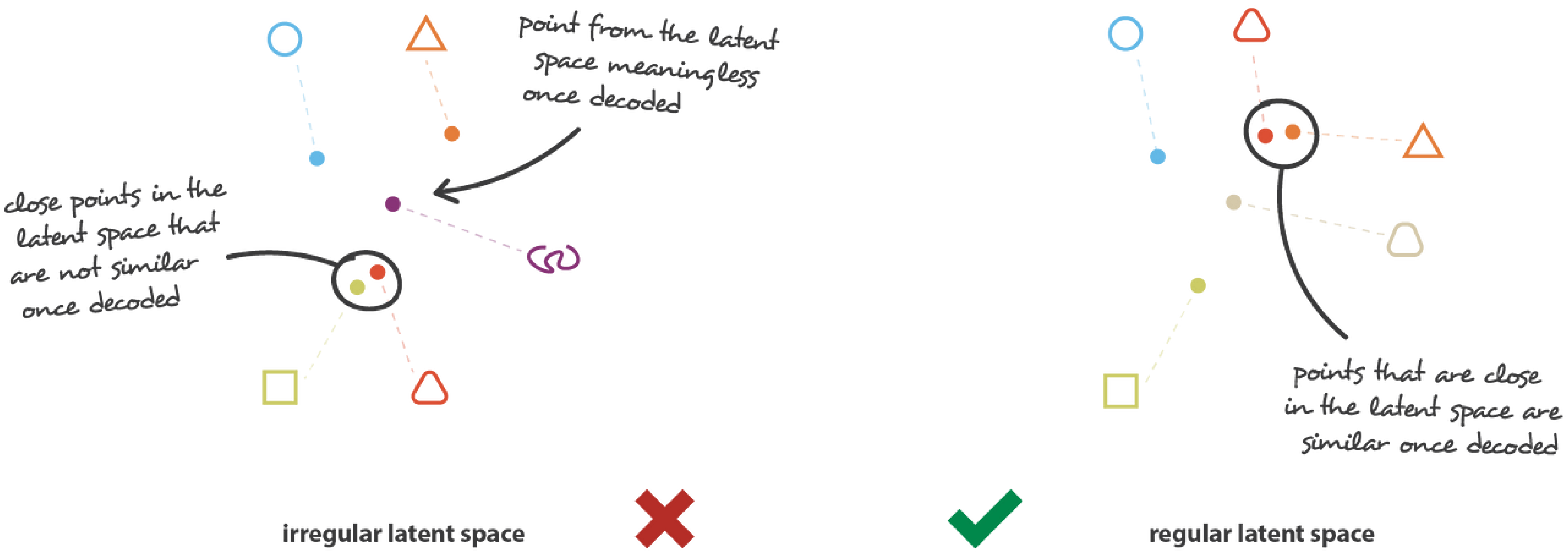

Can AEs learn such latent spaces that are good for reconstruction + generation? Yes, VAEs [7,8]!

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Maximum Likelihood

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

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Intractable Integration!

Evidence Lower Bound (ELBO)

Variational Approximation

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

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Integrating from both sides:

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Integrating from both sides:

Why is it a lower bound?

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$$= \int q_\phi(Z|X)\log\left(\frac{p_\theta(X,Z)}{q_\phi(Z|X)}\frac{q_\phi(Z|X)}{p_\theta(Z|X)}\right)dZ$$
$$= \int q_\phi(Z|X)\log\left(\frac{p_\theta(X,Z)}{q_\phi(Z|X)}\right)dZ + \int q_\phi(Z|X)\log\left(\frac{q_\phi(Z|X)}{p_\theta(Z|X)}\right)dZ$$
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Evidence Lower Bound (ELBO)

Variational Approximation

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

Integrating from both sides:

Why is it a lower bound? KL is nonnegative!

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

Evidence Lower Bound (ELBO)

Variational Approximation

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

Integrating from both sides:

Why is it a lower bound? KL is nonnegative!

Why is it called variational approximation?

$$
\begin{aligned}
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&= \int q_\phi(Z|X)\log\left(\frac{p_\theta(X,Z)}{q_\phi(Z|X)}\frac{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{\mathrm{KL}\left(q_\phi(Z|X)\|p_\theta(Z|X)\right)}_{\text{Kullback-Leibler (KL) Divergence}}
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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)

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

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ELBO:

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\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)}\left[\log\left(p_\theta(X|Z)\right)\right] + \mathbb{E}_{q_\phi(Z|X)}\left[\log\left(\frac{p_\theta(Z)}{q_\phi(Z|X)}\right)\right] \\
&= -\mathbb{E}_{q_\phi(Z|X)}\left[-\log\left(p_\theta(X|Z)\right)\right] - \mathrm{KL}\left(q_\phi(Z|X)\|p_\theta(Z)\right)
\end{aligned}$$

Evidence Lower Bound (ELBO)

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&= \underbrace{-\mathbb{E}_{q_\phi(Z|X)}\left[-\log\left(p_\theta(X|Z)\right)\right]}_{\text{Reconstruction Error/Loss}} - \underbrace{\mathrm{KL}\left(q_\phi(Z|X)\|p_\theta(Z)\right)}_{\text{Regularizer}}
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$$
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  - Motivation & Overview
  - Linear Autoencoders & PCA
  - Deep Autoencoders
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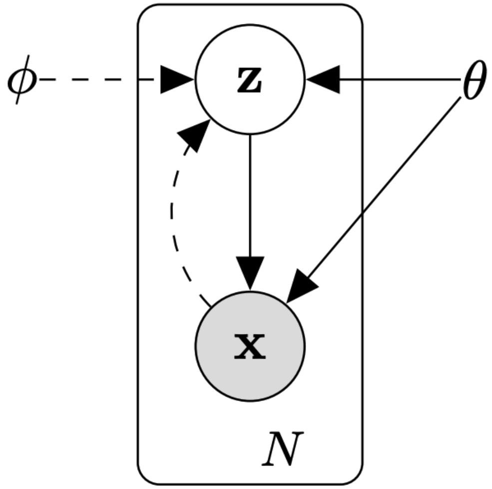
  - Evidence Lower Bound (ELBO)
  - **Models**
  - Amortized Inference
  - Reparameterization Trick
- Graph Variational Autoencoders

Variational Autoencoders

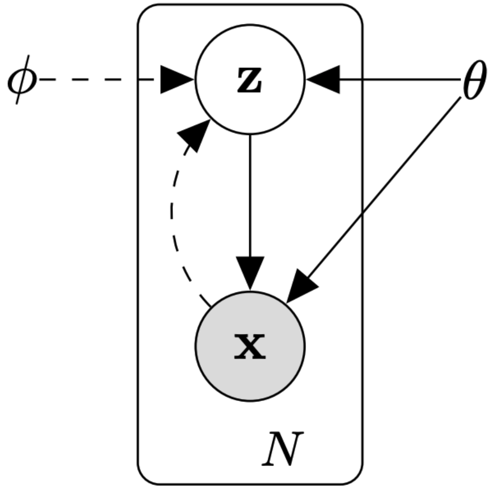


Encoder: $q_\phi(Z|X)$

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:

$$
\begin{aligned}
q_\phi(Z|X) &= \mathcal{N}(Z|\mu, \sigma^2 I) \\
\mu &= \mathrm{EncoderNetwork}_\phi(X) \\
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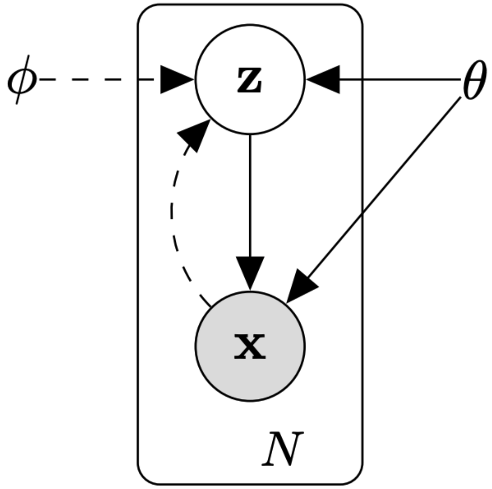
Variational Autoencoders



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Similarly, Gaussian distribution is often adopted for the decoder:

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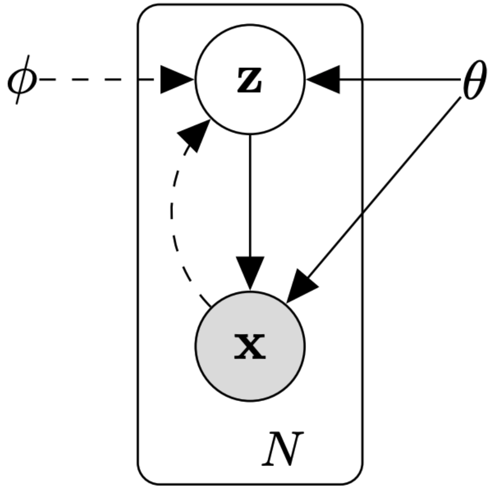
Variational Autoencoders



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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

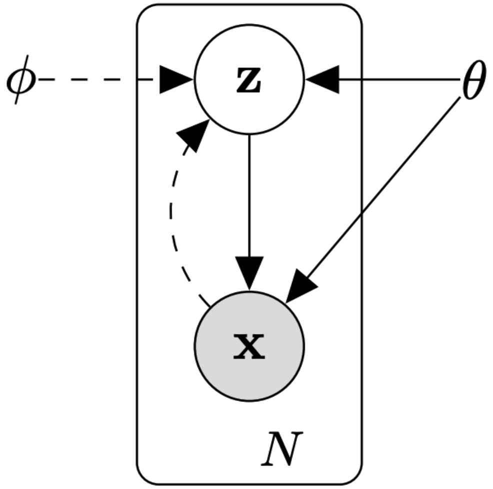

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Illustration of VAEs:

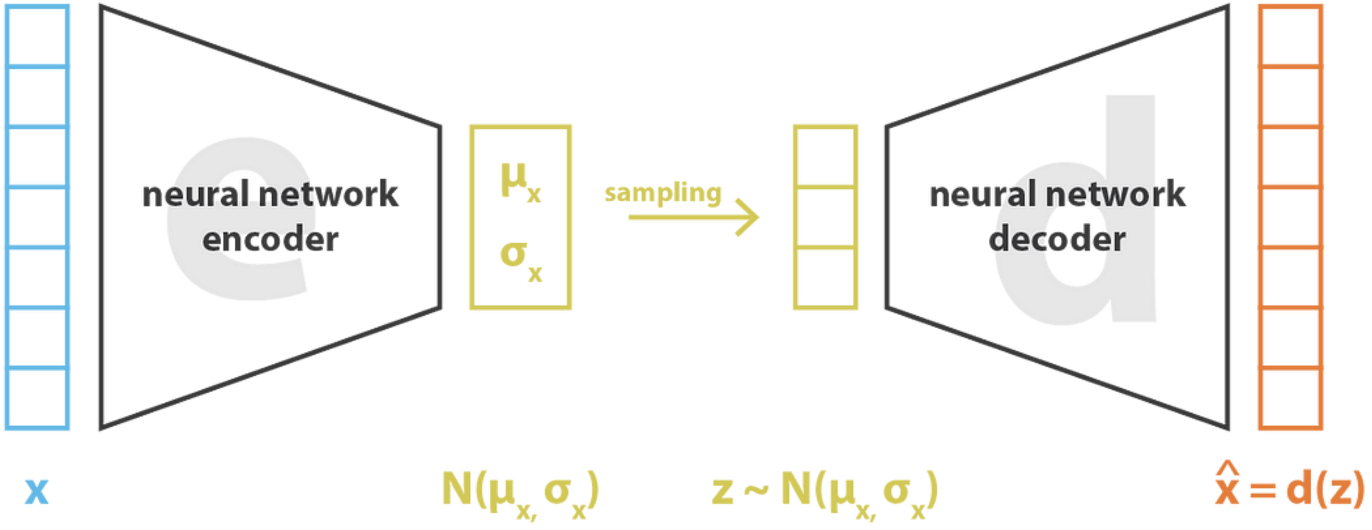

Image Credit: [6]

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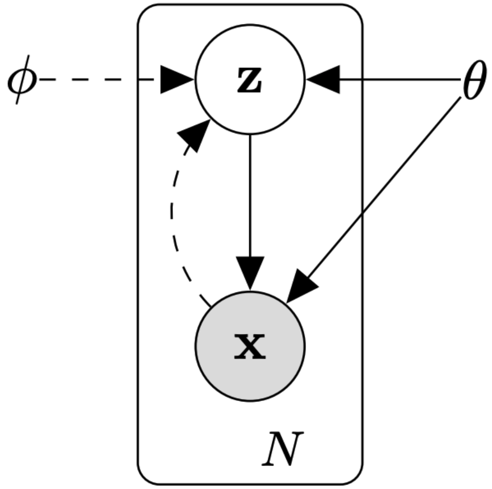
  - **Amortized Inference**
  - Reparameterization Trick
- Graph Variational Autoencoders

Amortized Variational Inference



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

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

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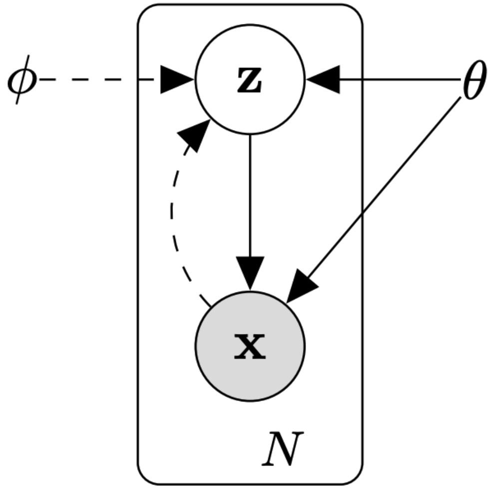
Amortized Variational Inference



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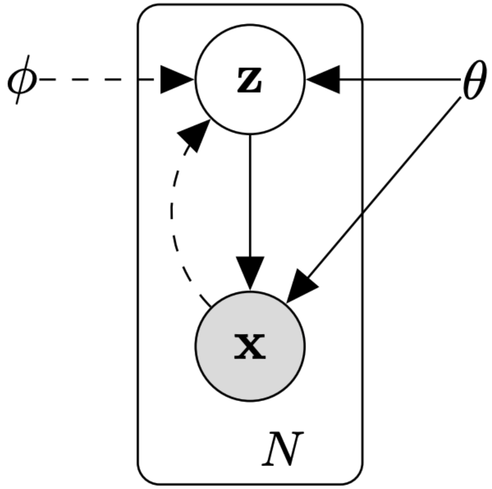
We thus only need to optimize ELBO over one set of parameters ϕ, whereas in traditional variational inference (VI) one needs to find the optimal variational distribution per X

Amortized Variational Inference



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

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- Graph Variational Autoencoders

Reparameterization Trick

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

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

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

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$$\approx -\frac{1}{N}\sum_{\substack{i=1 \\ Z_i\sim q_\phi(Z|X)}}^{N} \log\left(p_\theta(X|Z_i)\right) + \mathrm{KL}\left(q_\phi(Z|X)\|p_\theta(Z)\right)$$

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Gradient of the decoder (assuming prior is not learnable for simplicity) [7]:

$$\begin{aligned}\frac{\partial \mathcal{L}(\phi, \theta)}{\partial \theta} &= \mathbb{E}_{q_\phi(Z|X)}\left[-\frac{\partial \log\left(p_\theta(X|Z)\right)}{\partial \theta}\right] \\ &\approx -\frac{1}{N} \sum_{\substack{i=1 \\ Z_i \sim q_\phi(Z|X)}}^{N} \frac{\partial \log\left(p_\theta(X|Z_i)\right)}{\partial \theta}\end{aligned}$$

Reparameterization Trick

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

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

Once we draw samples of Z, we can get the Monte Carlo gradient of reconstruction loss w.r.t. θ via backpropagation

We will use *reparameterization trick (a.k.a. pathwise derivatives)* to equivalently rewrite the expectation in reconstruction loss so that the Monte Carlo gradient w.r.t. ϕ has a low variance.

Reparameterization Trick

For any function f, we have

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

Change of Variable

Reparameterization Trick

For any function f, we have

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

Change of Variable

Therefore,

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

Reparameterization Trick

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

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

where

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

Reparameterization Trick

Therefore, in original VAE, we have

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

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Therefore, in original VAE, we have

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

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

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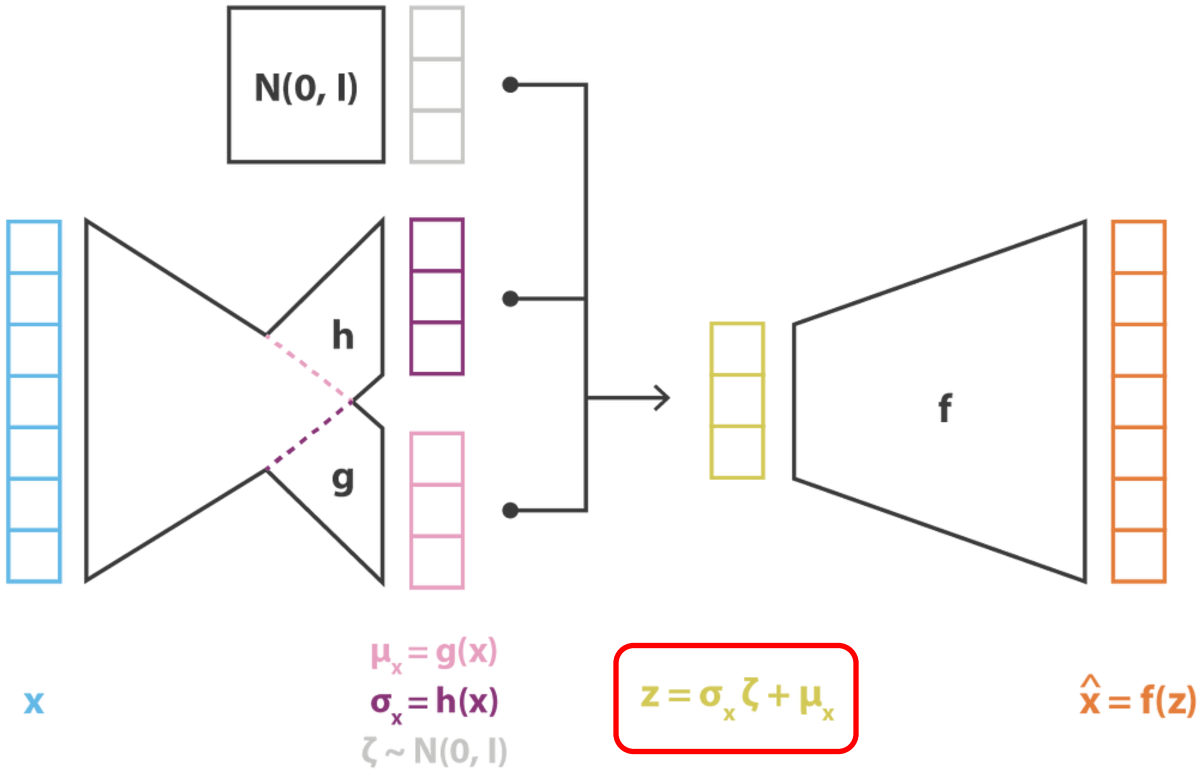
Now we can get the gradient directly!

Reparameterization Trick

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



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

Image Credit: [6]

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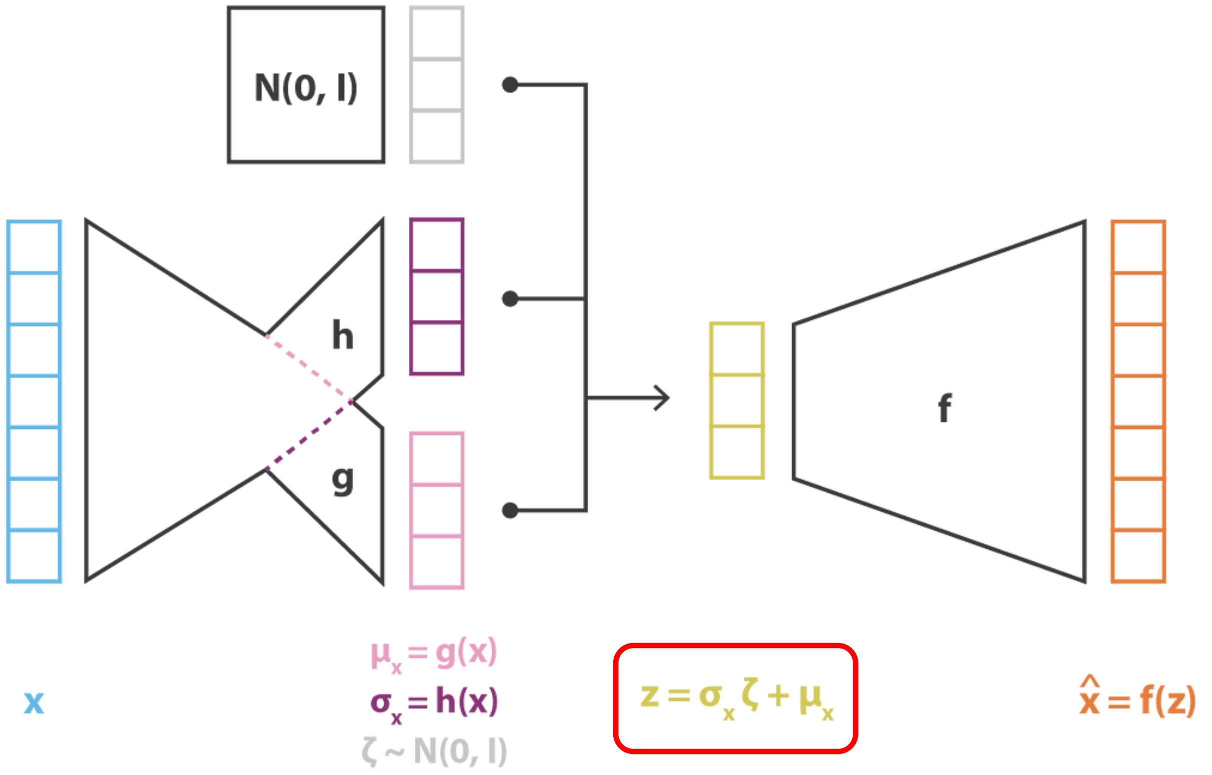

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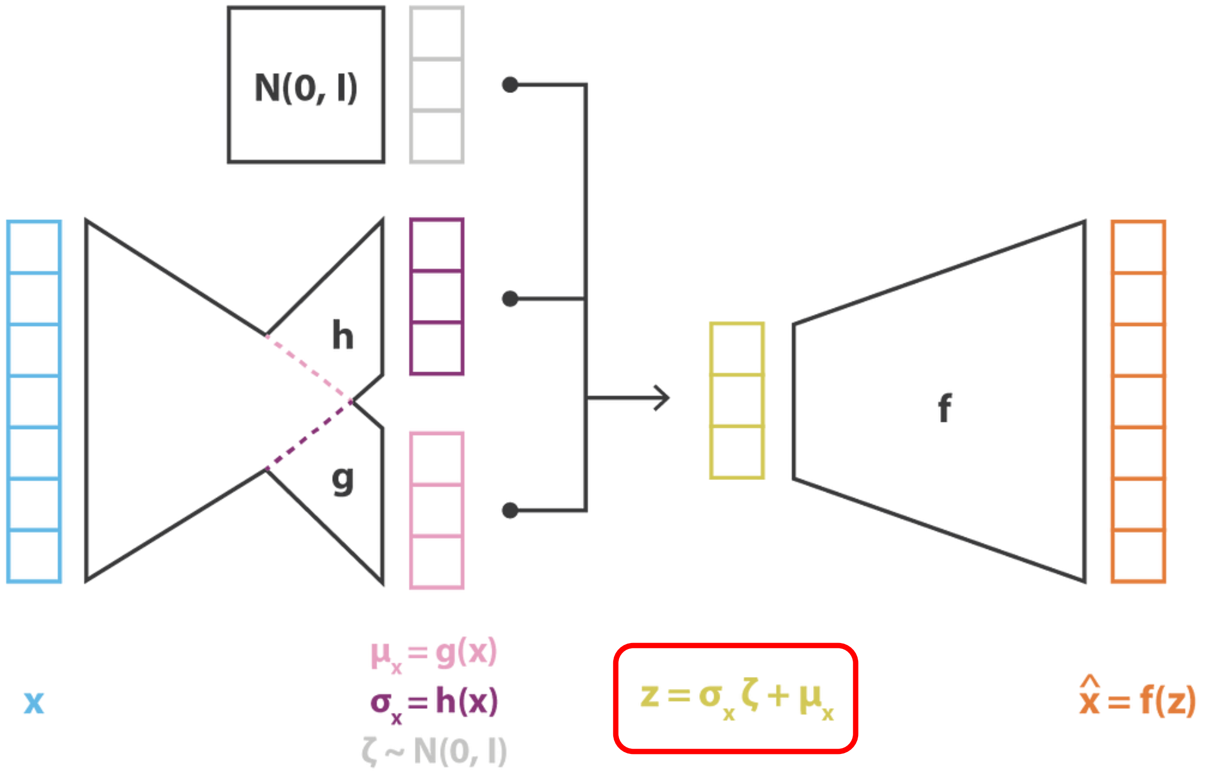
What if we have discrete latent variables in VAEs?

Image Credit: [6]

Reparameterization Trick

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



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

What if we have discrete latent variables in VAEs?

Reparameterization trick does not work exactly since sampling path is non-differentiable!

Image Credit: [6]

Reparameterization Trick

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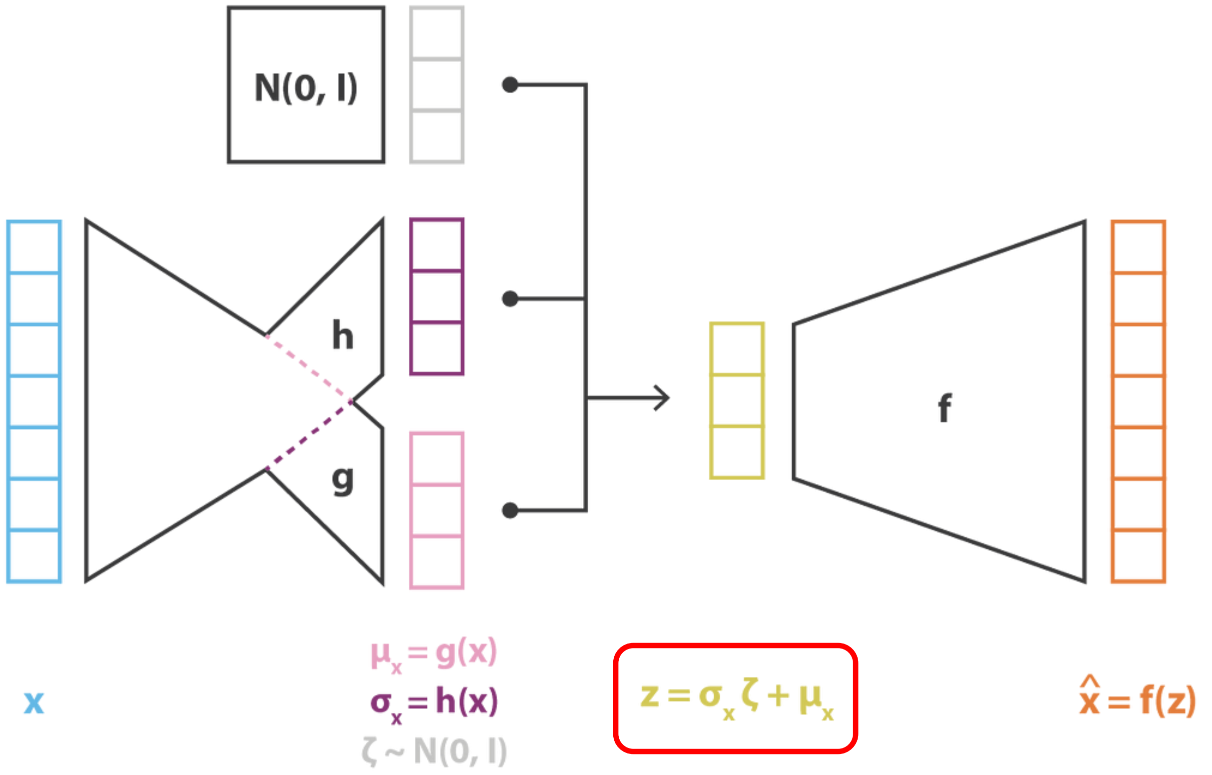

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What if we have discrete latent variables in VAEs?

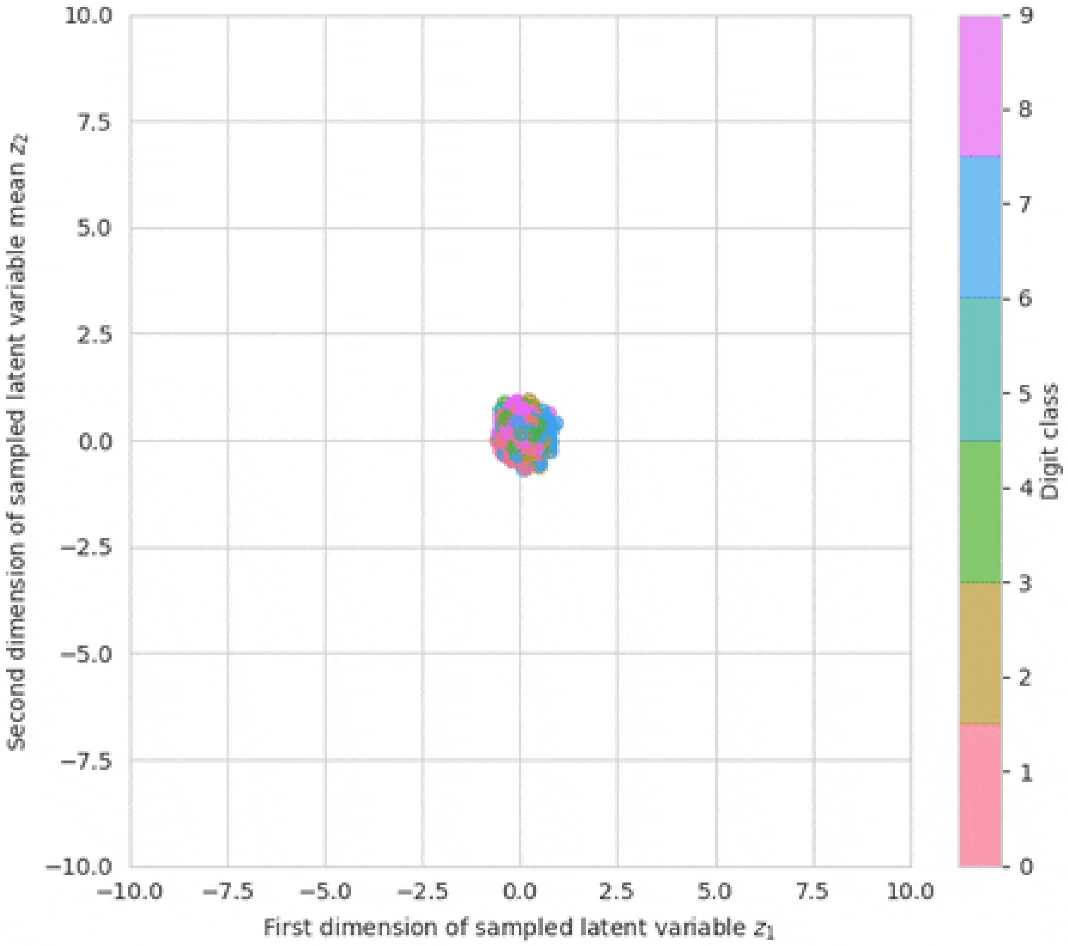
Reparameterization trick does not work exactly since sampling path is non-differentiable!

We need *Monte Carlo gradient estimation* methods which are covered by a separate lecture.

Image Credit: [6]

VAEs on MNIST

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



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

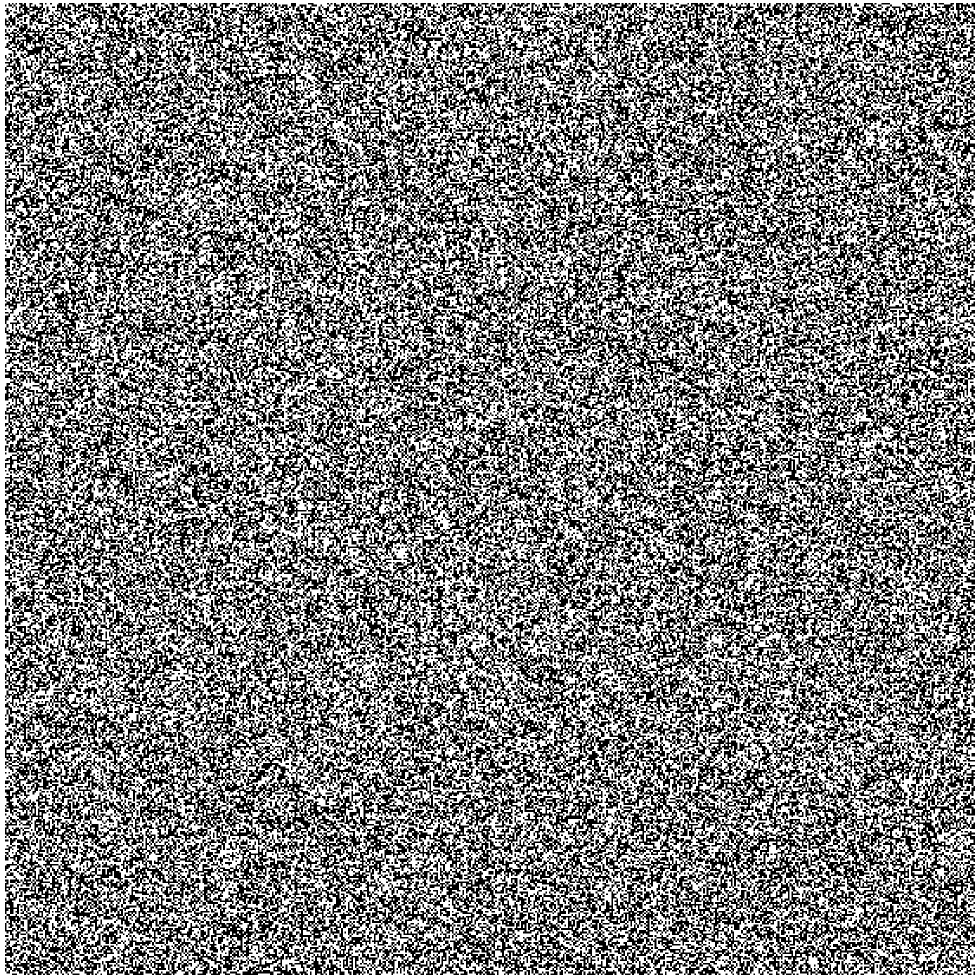


Image Credit: [9]

Outline

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

Graph Variation Autoencoders

Graph VAEs [10, 11] generalize VAEs to graph structured data:

Node feature:	$X \in \mathbb{R}^{n \times d}$
Node latent variables:	$Z \in \mathbb{R}^{n \times m}$
Adjacency matrix:	$A \in \mathbb{R}^{n \times n}$

Graph Variation Autoencoders

Graph VAEs [10, 11]:

Encoder:

$$\begin{aligned} q_\phi(Z|X,A) &= \prod_i q_\phi(Z_i|X,A) \\ q_\phi(Z_i|X,A) &= \mathcal{N}(Z_i|\mu_i, \sigma_i^2 I) \\ H &= \mathrm{GNN}_\phi(X,A) \\ \mu_i, \log\sigma_i^2 &= \mathrm{Readout}_\phi(H) \end{aligned}$$

Graph Variation Autoencoders

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Prior:

$$p(Z) = \prod_i p(Z_i) = \prod_i \mathcal{N}(Z_i|0, I)$$

Graph Variation Autoencoders

Graph VAEs [10, 11]:

Decoder: $$p_\theta(X, A|Z) = p_\theta(A|Z)p_\theta(X|A, Z)$$

Graph Variation Autoencoders

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Adjacency Matrix Decoder:

$$p_\theta(A|Z) = \prod_i \prod_j p_\theta(A_{ij}|Z)$$

$$H = \mathrm{MLP}(Z)$$

$$p_\theta(A_{ij} = 1|Z_i, Z_j) = \sigma(H_i^\top H_j)$$

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Node Feature Decoder:

$$p_\theta(X|A, Z) = \prod_i p_\theta(X_i|A, Z)$$

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

$$\tilde{H} = \mathrm{GNN}_\theta(Z, A)$$

$$\tilde{\mu}_i, \log \tilde{\sigma}_i^2 = \mathrm{Readout}_\theta(\tilde{H})$$

Graph Variation Autoencoders

Graph VAEs [10, 11]:

Learning:

$$\begin{aligned}\log p_\theta(X, A) &\geq \mathrm{ELBO} \\ &= -\mathbb{E}_{q_\phi(Z|A,X)}\left[-\log\left(p_\theta(X, A|Z)\right)\right] - \mathrm{KL}\left(q_\phi(Z|X, A) \| p_\theta(Z)\right)\end{aligned}$$

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$$

Are we done?

Graph Variation Autoencoders

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Are we done?

No! We hope ELBO is permutation invariant!

Graph Variation Autoencoders

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Recall we use GNN as the encoder and the encoder is conditional independent

$$\begin{aligned}q_\phi(Z|X, A) &= \prod_i q_\phi(Z_i|X, A) \\ q_\phi(Z_i|X, A) &= \mathcal{N}(Z_i|\mu_i, \sigma_i^2 I) \\ H &= \text{GNN}_\phi(X, A) \\ \mu_i, \log\sigma_i^2 &= \text{Readout}_\phi(H)\end{aligned}$$

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Recall we use GNN as the encoder and the encoder is conditional independent, we have

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Encoder is permutation invariant!

$$\forall P \in \Pi \qquad q_\phi(Z|PAP^\top, PX) = q_\phi(Z|A, X)$$

Graph Variation Autoencoders

Graph VAEs [10, 11]:

Learning:

$$
\begin{aligned}
\log p_\theta(X, A) &\geq \text{ELBO} \\
&= -\mathbb{E}_{q_\phi(Z|A,X)}\left[-\log\left(p_\theta(X, A|Z)\right)\right] - \text{KL}\left(q_\phi(Z|X, A) \| p_\theta(Z)\right)
\end{aligned}
$$

Similarly, recall we use GNN as the decoder and the decoder is conditional independent, we have

Decoder is permutation invariant!

$$
\forall P \in \Pi \qquad p_\theta(PAP^\top, PX|PZ) = p_\theta(X, A|Z)
$$

Graph Variation Autoencoders

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\end{aligned}
$$

Similarly, recall we use GNN as the decoder and the decoder is conditional independent, we have

Decoder is permutation invariant!

$$
\forall P \in \Pi \qquad p_\theta(PAP^\top, PX|PZ) = p_\theta(X, A|Z)
$$

And prior is standard multivariate Normal, which is permutation invariant.

Therefore, the ELBO is permutation invariant!

Graph Variation Autoencoders

Graph VAEs [10, 11]:

If you use a permutation invariant encoder or decoder, ELBO is not longer invariant.

How to approximately achieve permutation-invariance?

Graph Variation Autoencoders

Graph VAEs [10, 11]:

If you use a permutation invariant encoder or decoder, ELBO is not longer invariant.

How to approximately achieve permutation-invariance?

- Sample a few random permutations
  (e.g., importance sampling, special permutations from domain knowledge)

$$
\begin{aligned}
\log\left(\sum_{P\in\Pi} p_\theta(PX, PAP^\top)\right) &\geq \log\left(\sum_{P\in S} p_\theta(PX, PAP^\top)\right) \\
&= \log\left(\sum_{P\in S} \exp\left(\log p_\theta(PX, PAP^\top)\right)\right) \\
&\geq \log\left(\sum_{P\in S} \exp\left(\mathrm{ELBO}\right)\right)
\end{aligned}
$$

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Questions?