EECE 571F: Deep Learning with Structures

Lecture 8 II: Auto-Encoders & Variational Auto-Encoders

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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

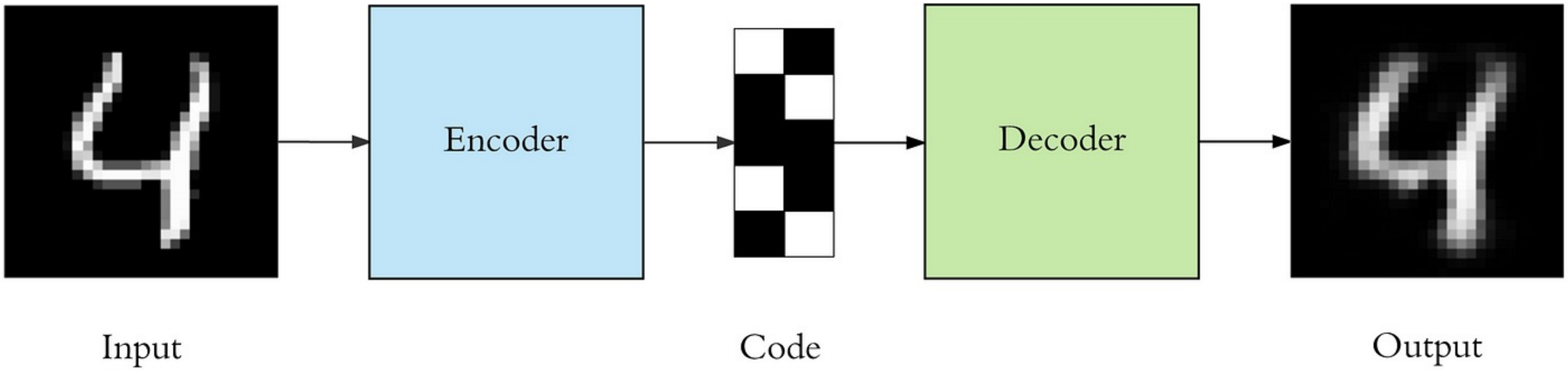

Image Credit: [1]

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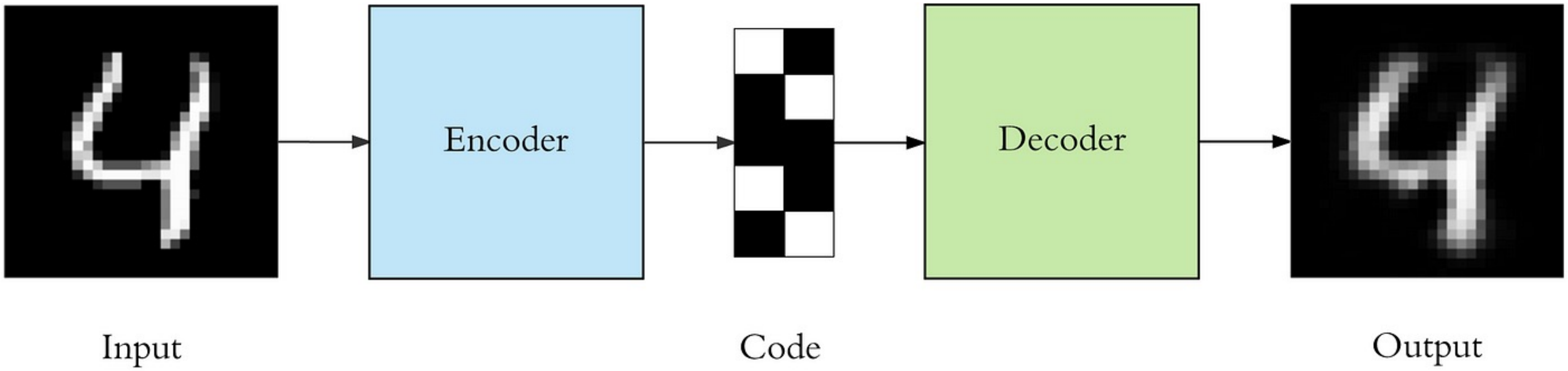
- To make it non-trivial, we need a *bottleneck* (i.e. the dimension of code being much smaller compared to the input). Why?



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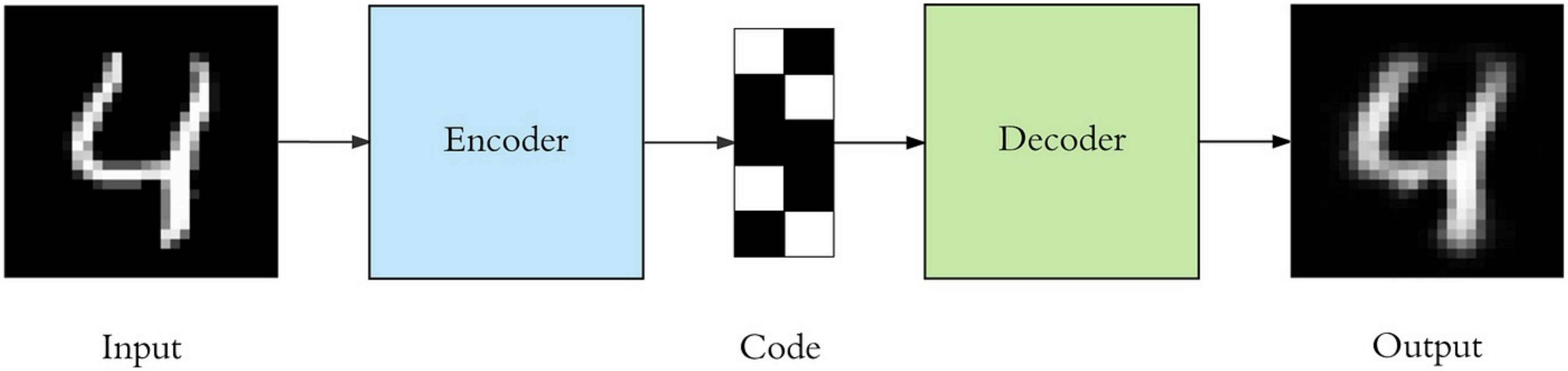

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Why should we care?

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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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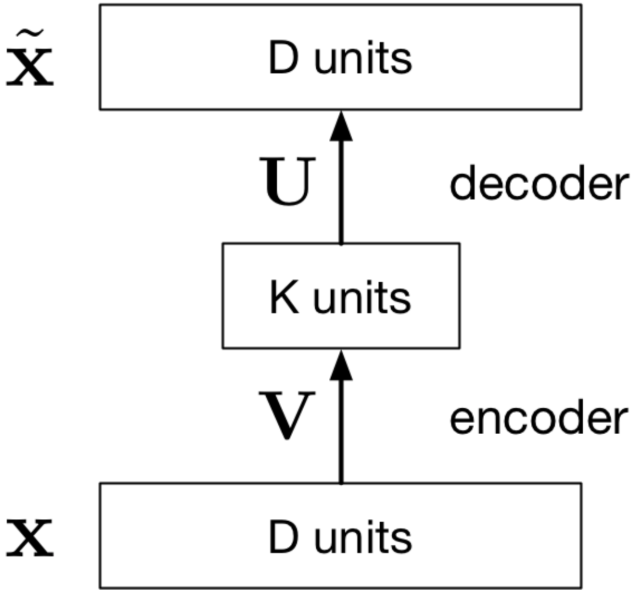
Linear Autoencoders

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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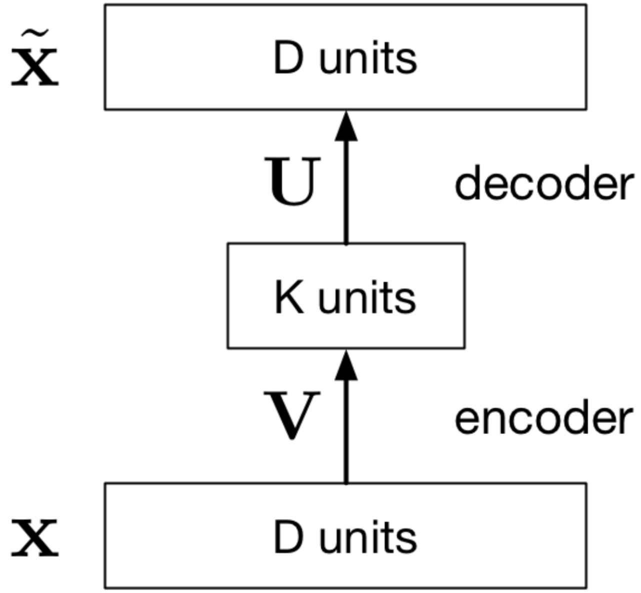

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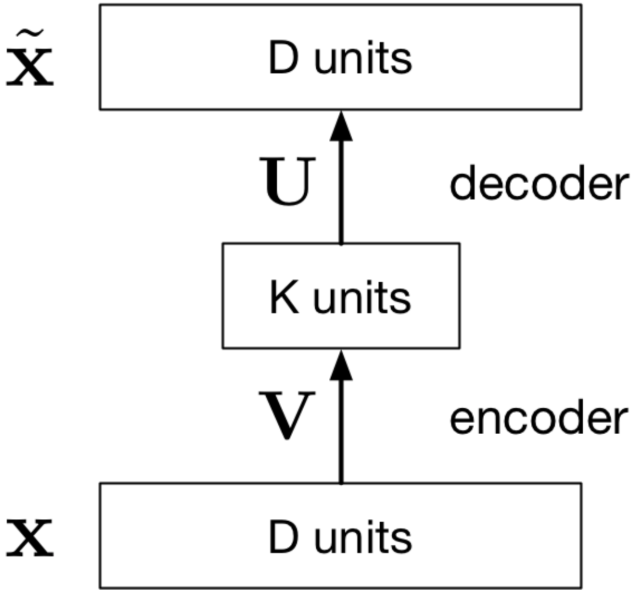

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Underdetermined system of equations, possibly having infinite solutions

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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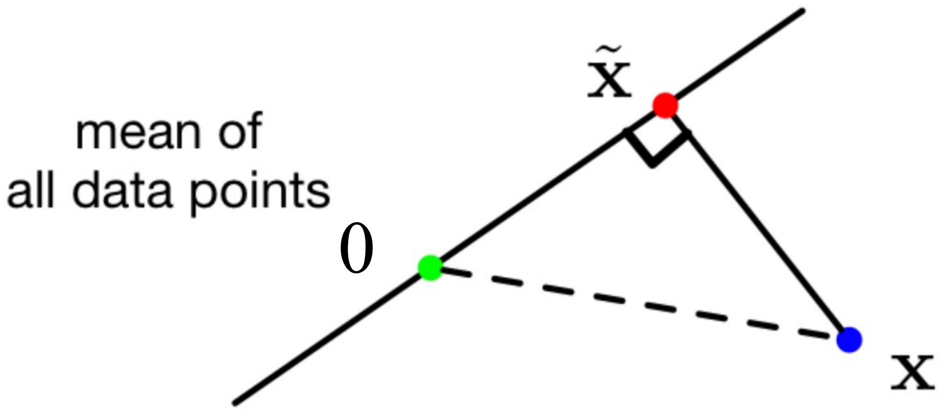
By Pythagorean Theorem, we have:

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



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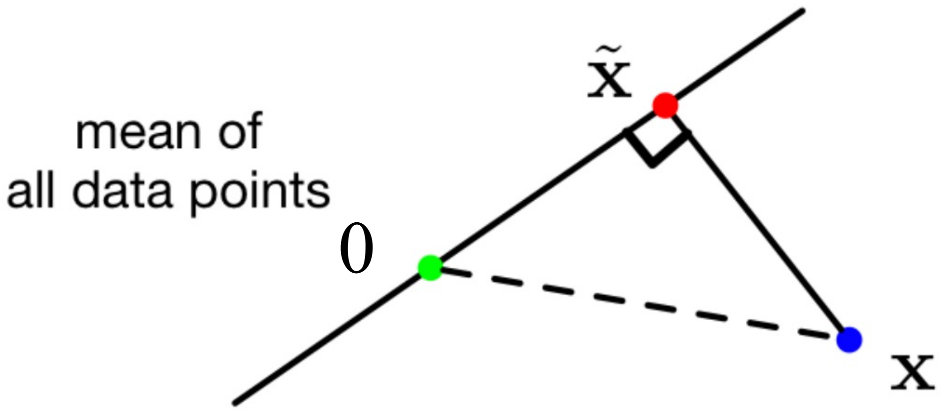

Maximizing the projected variance is equivalent to minimizing the reconstruction error!

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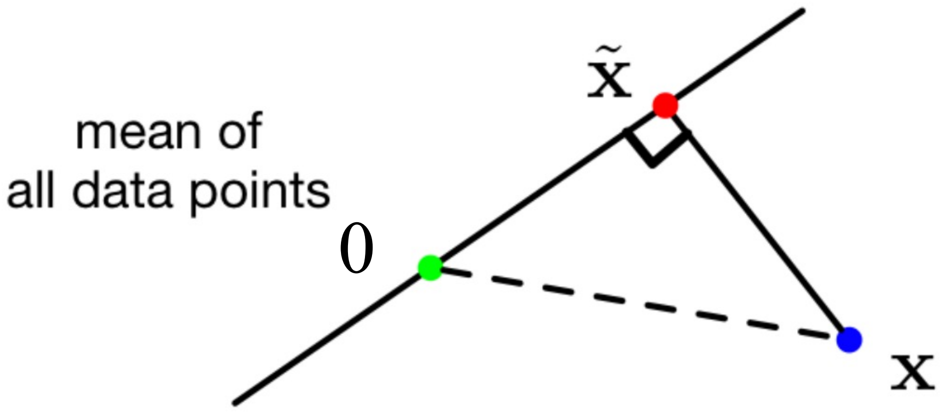

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Maximizing the projected variance is equivalent to minimizing the reconstruction error!

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

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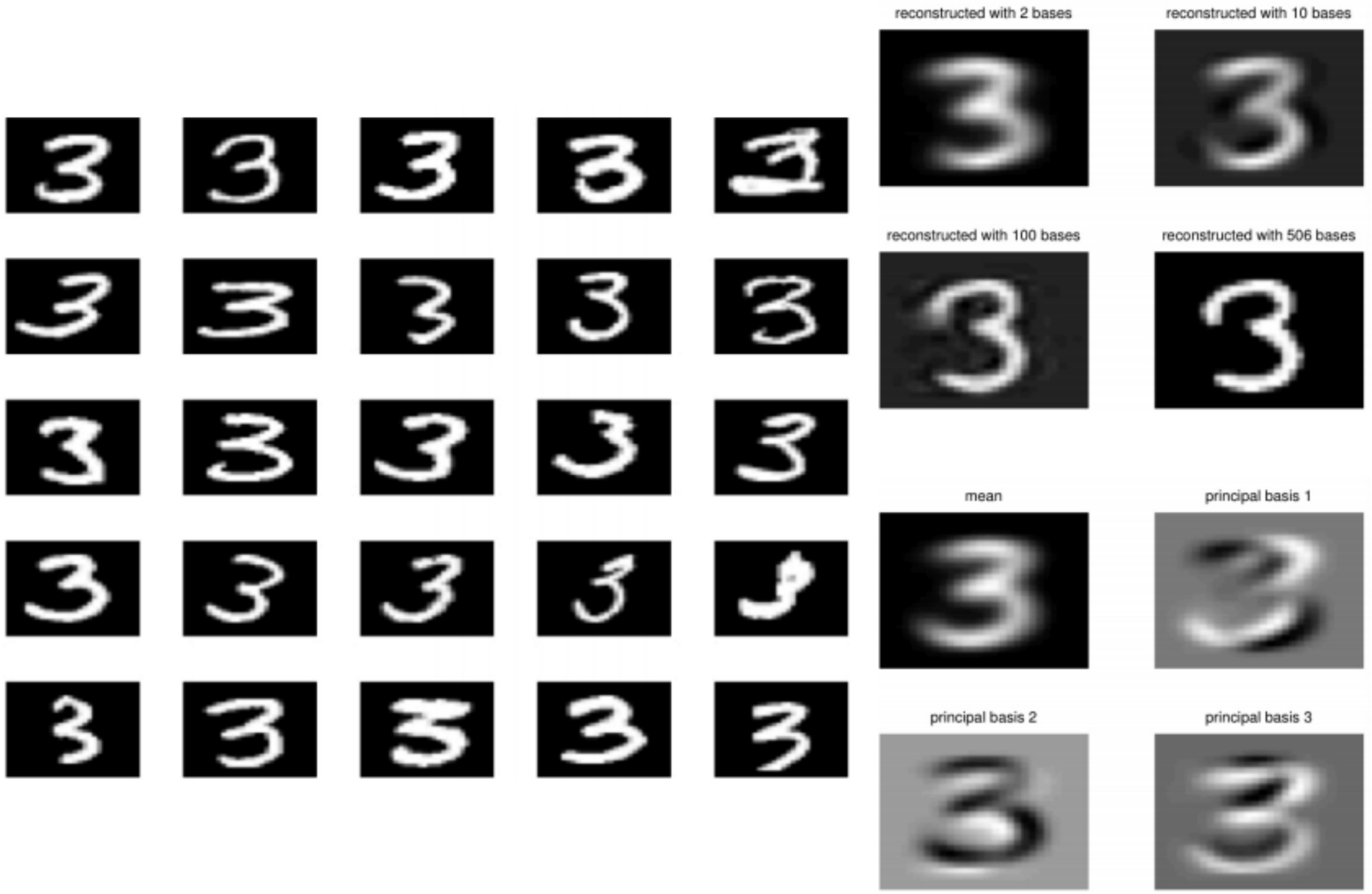
Principle components of faces ("Eigenfaces") from CBCL dataset:

Image Credit: [2]

Linear Autoencoders & Principle Component Analysis

Principle components of digits from MNIST dataset:



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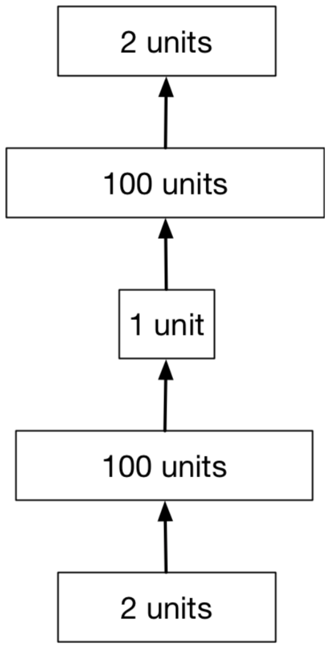
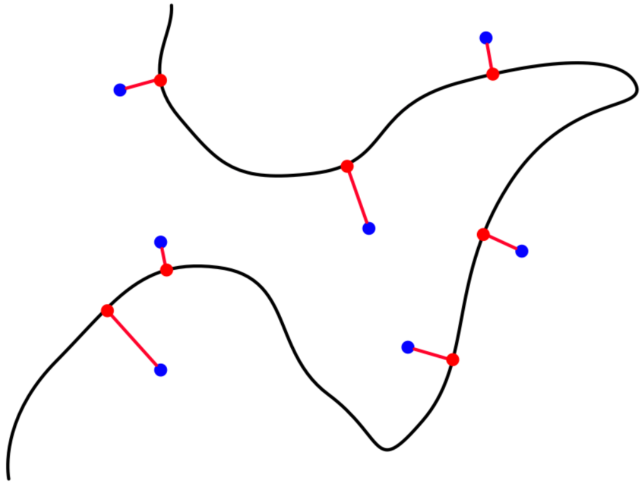
Deep Autoencoders

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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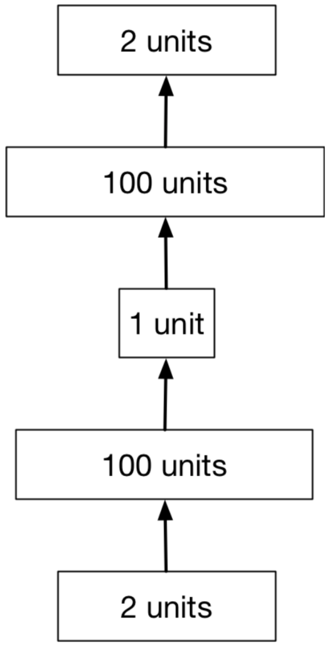

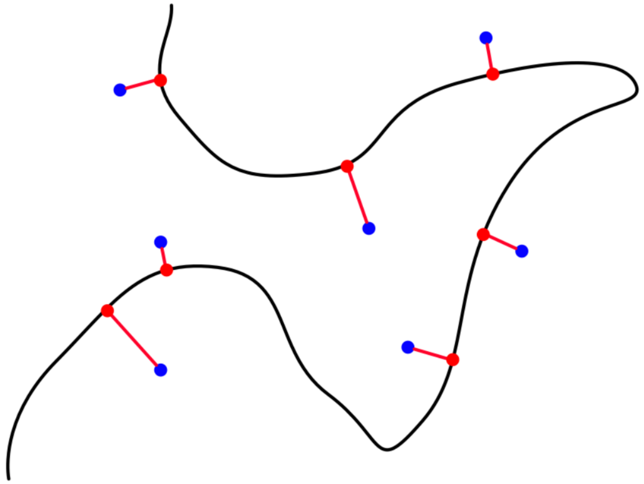

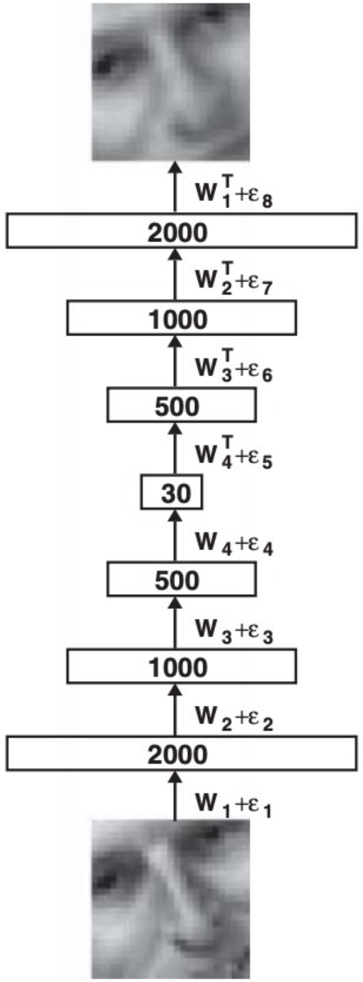

Image Credit: [2,4]

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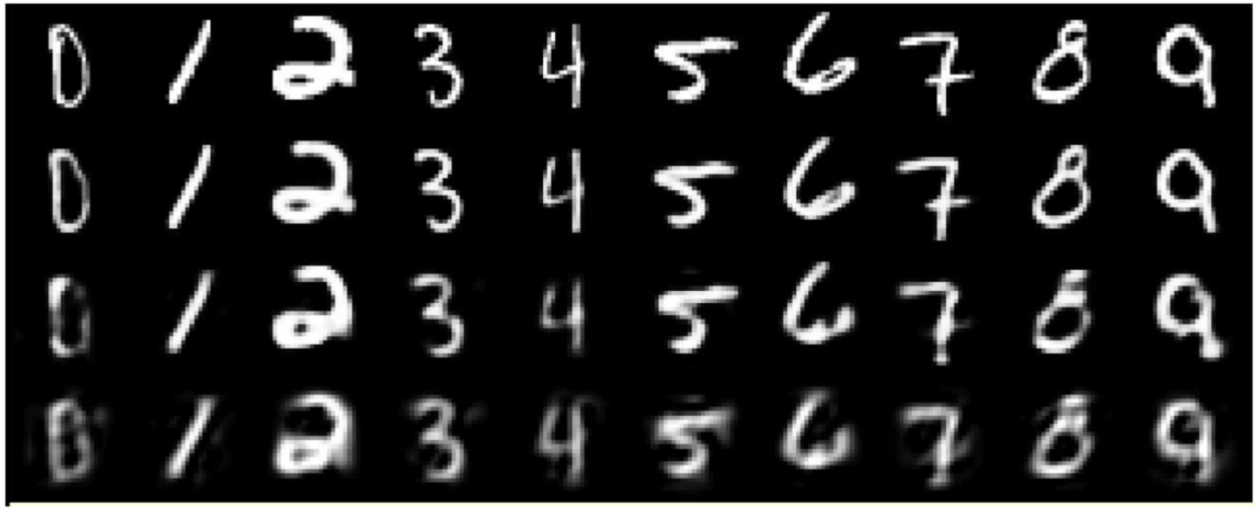
Deep autoencoders can learn more powerful codes/representations compared to linear ones (PCA)

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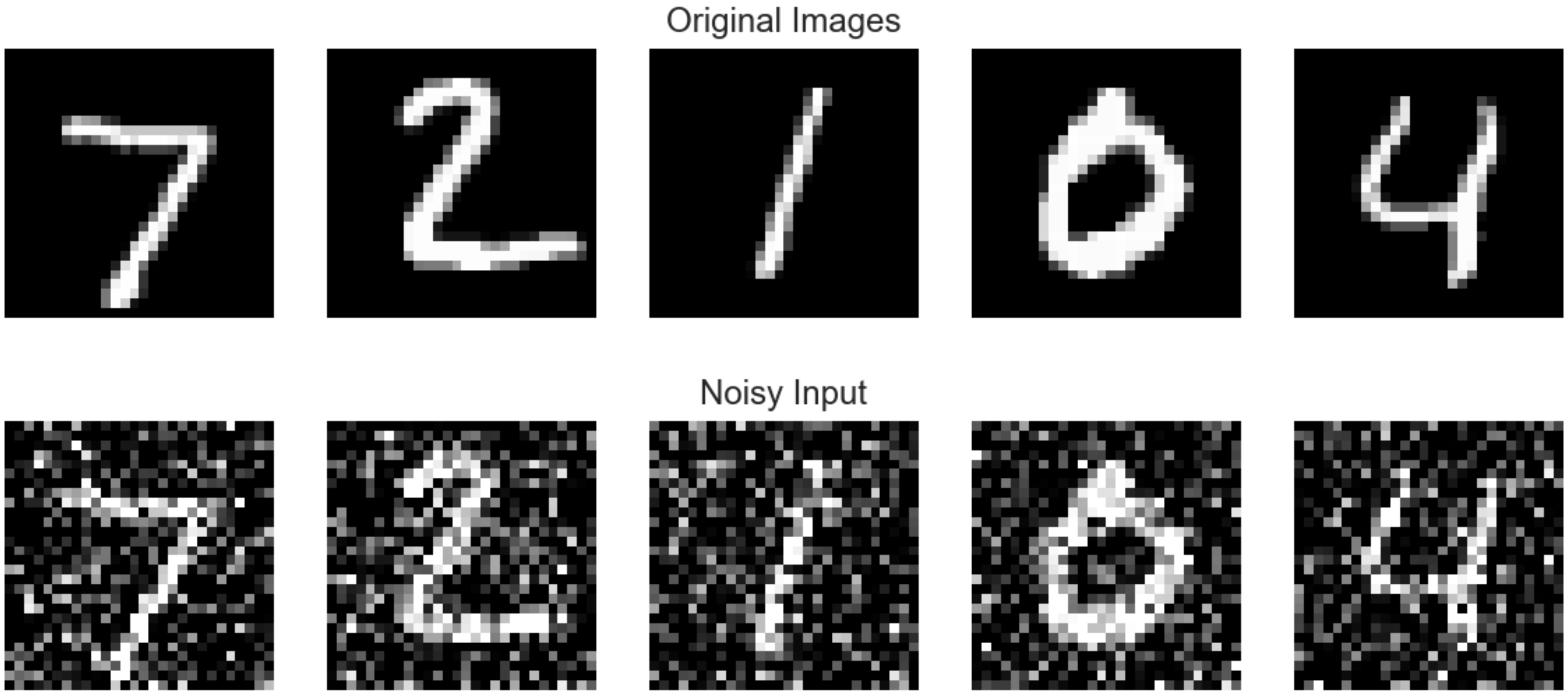
We can also achieve a similar goal via **denoising**!



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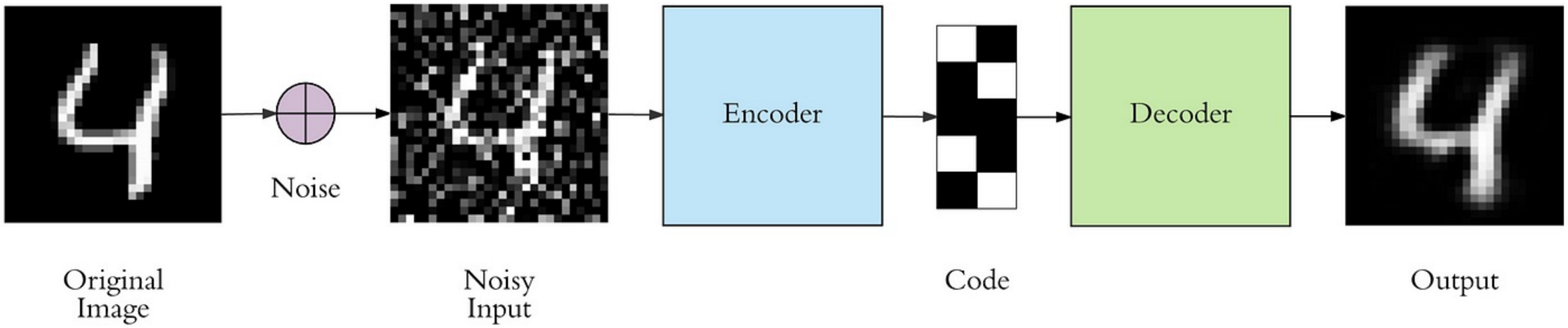
We add random noise (e.g., additive Gaussian) and force the neural network to learn useful representations so that *structures in images are preserved whereas noise is removed!*



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Denoising Autoencoders (DAEs)

DAEs can do a great job in denoising:

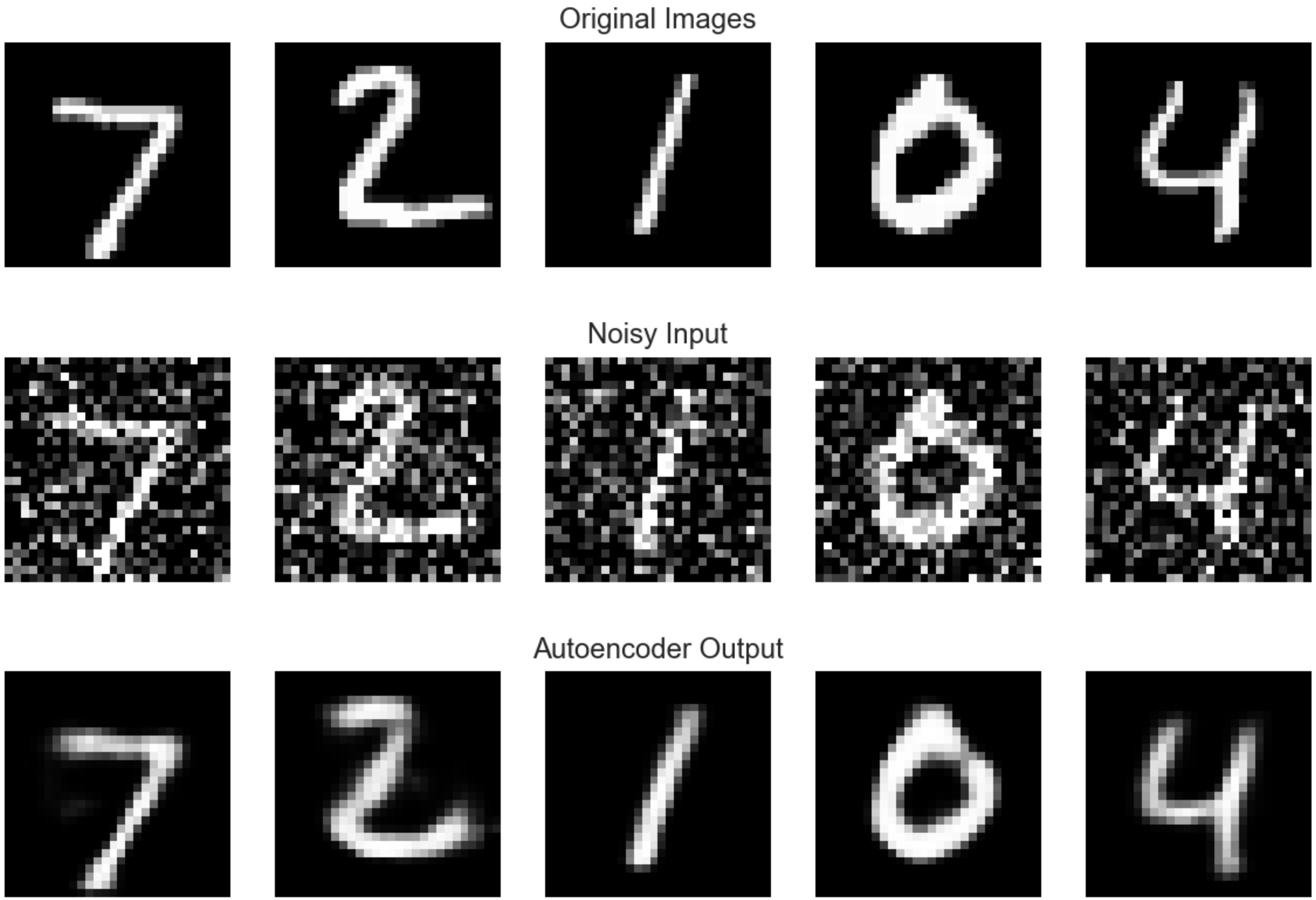
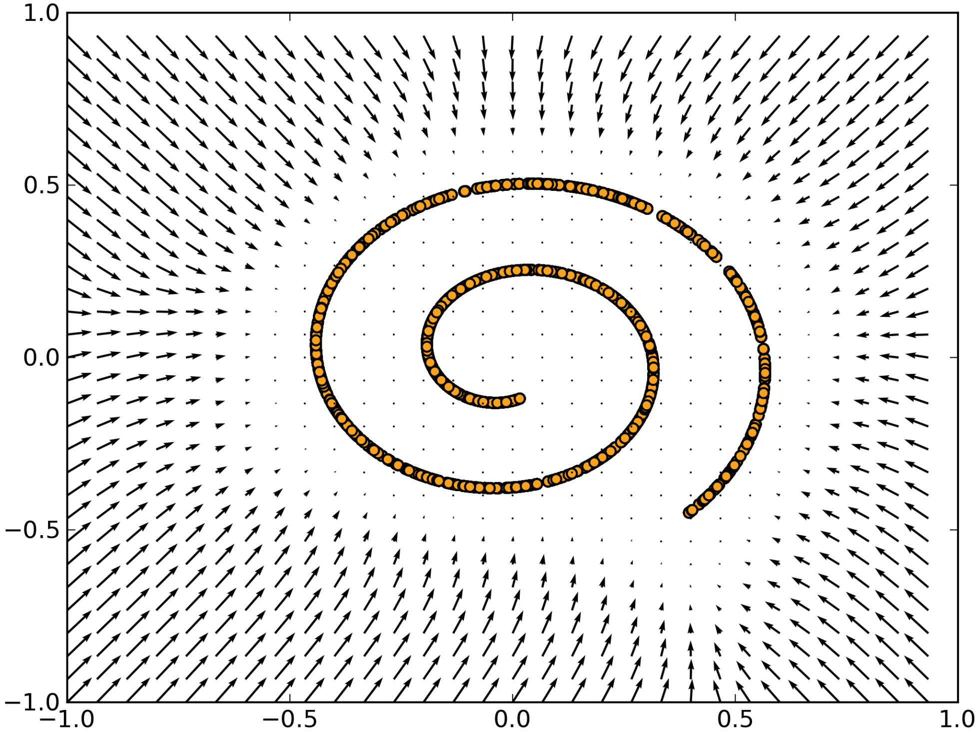


Image Credit: [1]

Denoising Autoencoders (DAEs)

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



zoom out

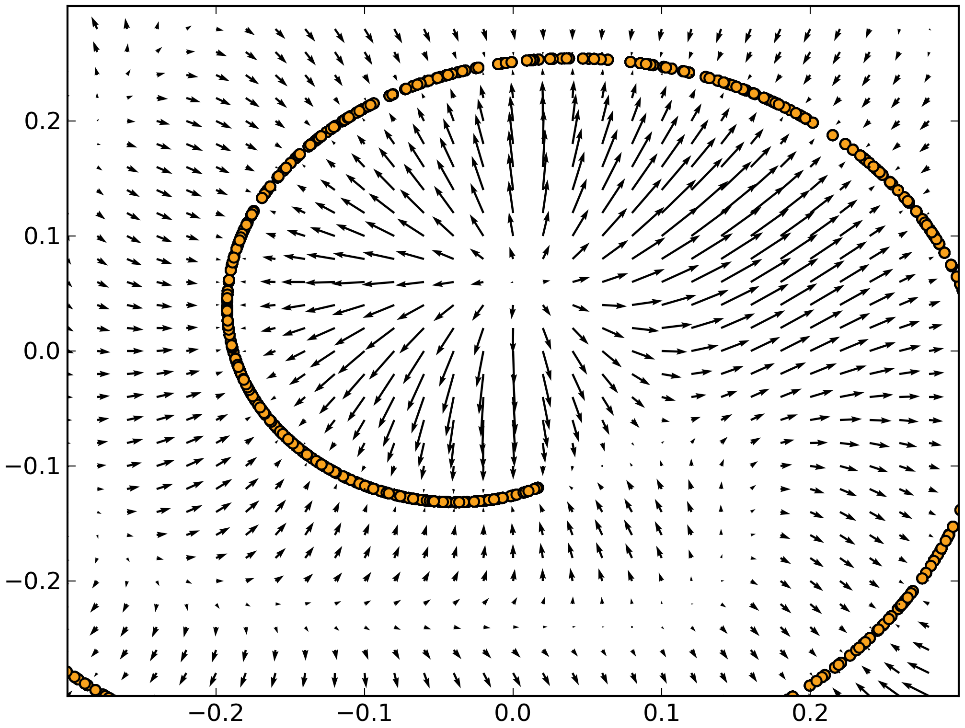


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Image Credit: [5]

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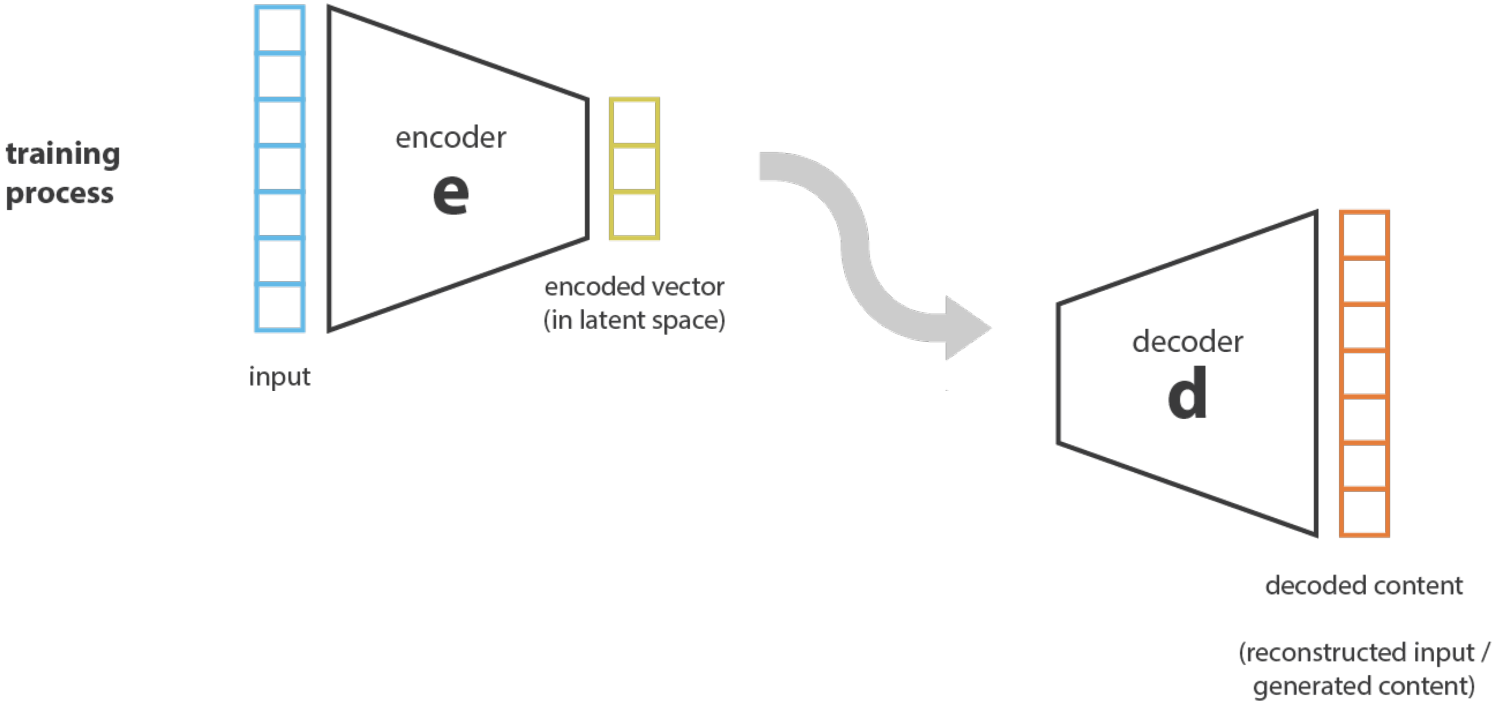

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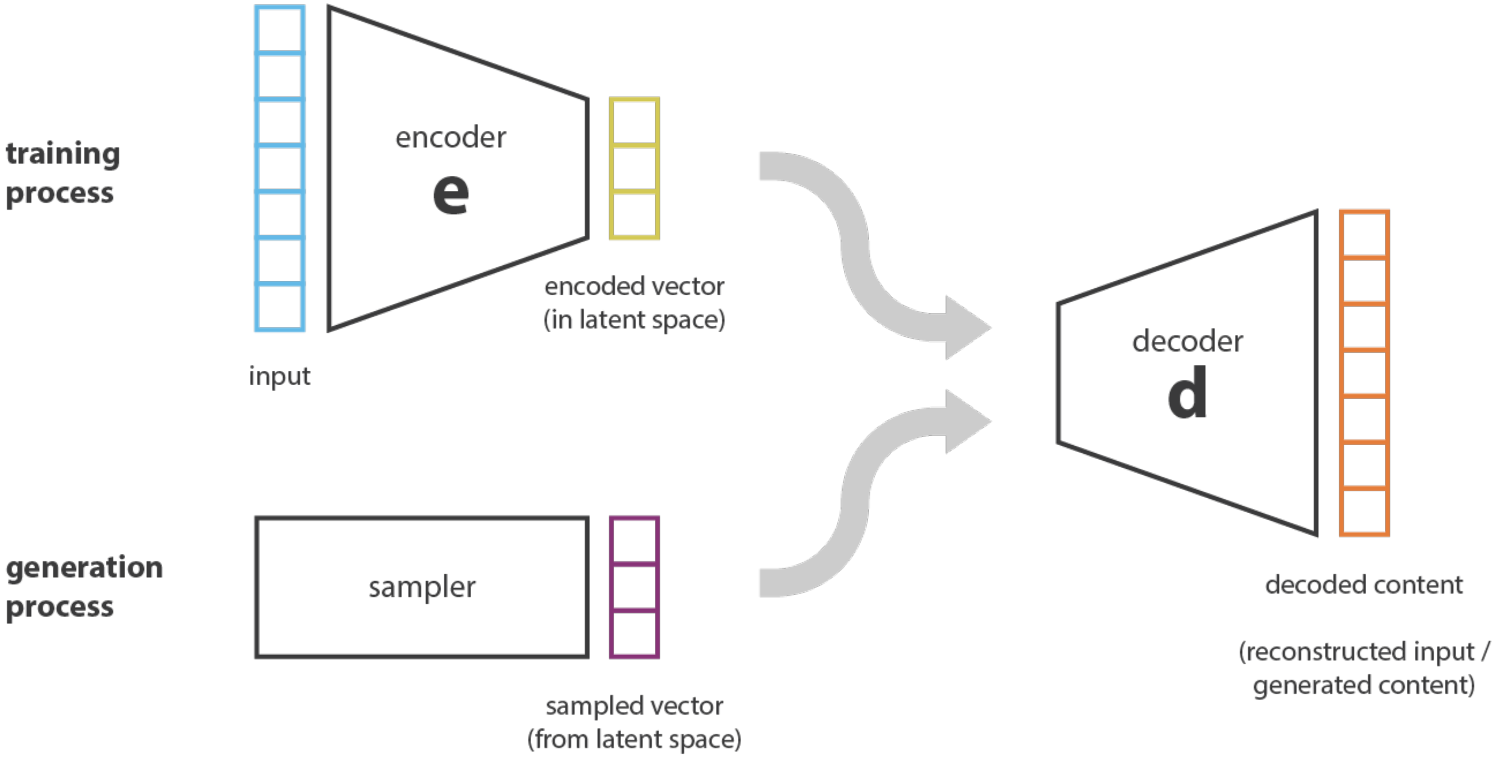

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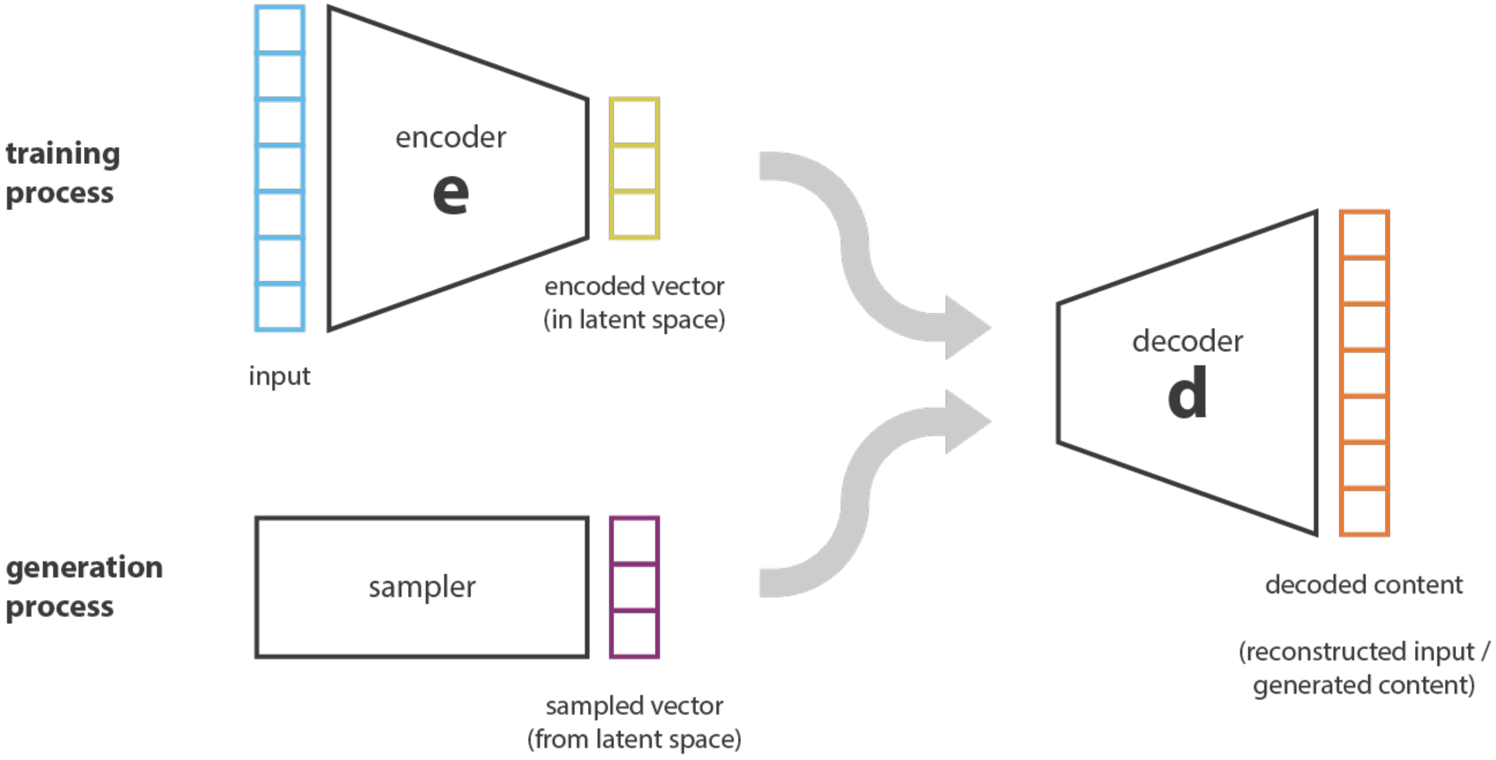

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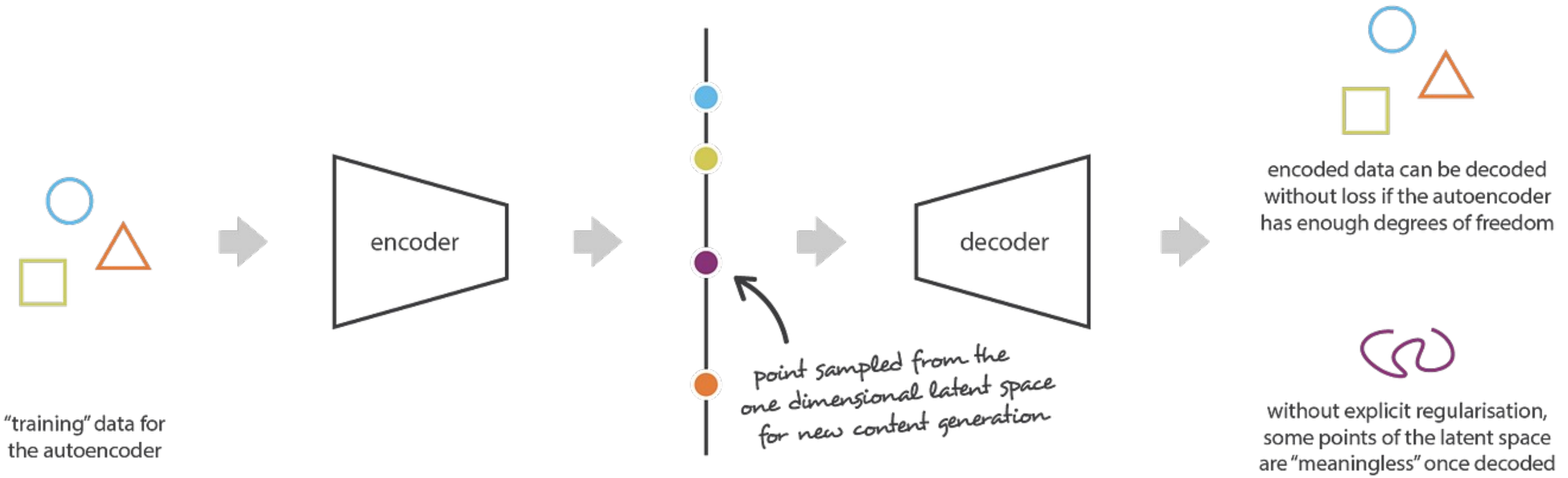
What would happen? *Sampled data could be very bad if sampled latent codes are far off the manifold!*



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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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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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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)   Kullback-Leibler (KL) Divergence

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!

Why is it called variational approximation?

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

Evidence Lower Bound (ELBO)

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

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

Evidence Lower Bound (ELBO)

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ELBO:

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

Evidence Lower Bound (ELBO)

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

ELBO:

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

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\end{aligned}$$

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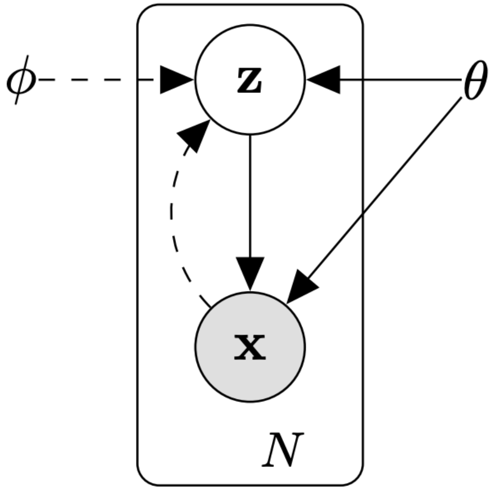
  - **Models**
  - Amortized Inference
  - Reparameterization Trick
- Graph Variational Autoencoders

Variational Autoencoders

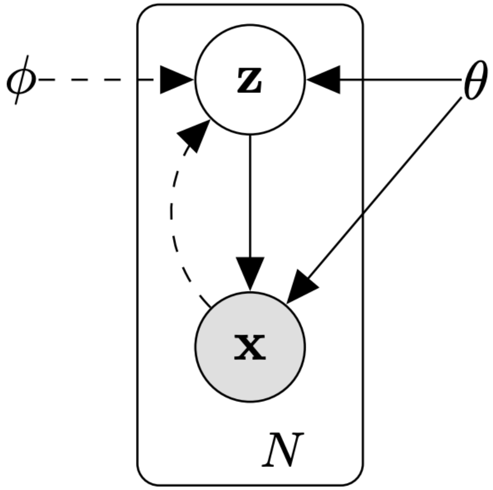


Encoder: $q_\phi(Z|X)$

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:

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

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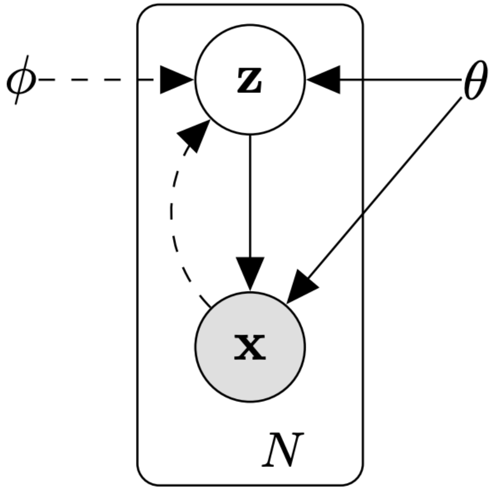
Variational Autoencoders



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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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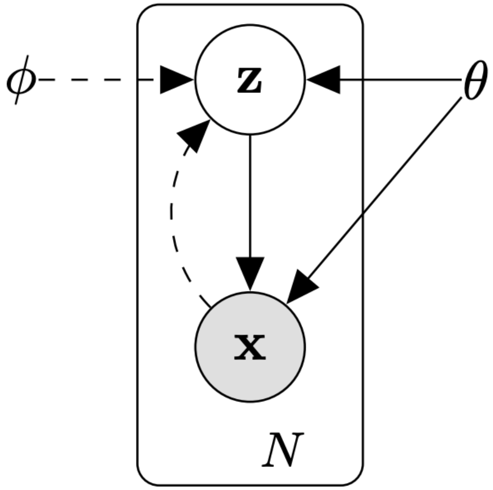
Variational Autoencoders



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

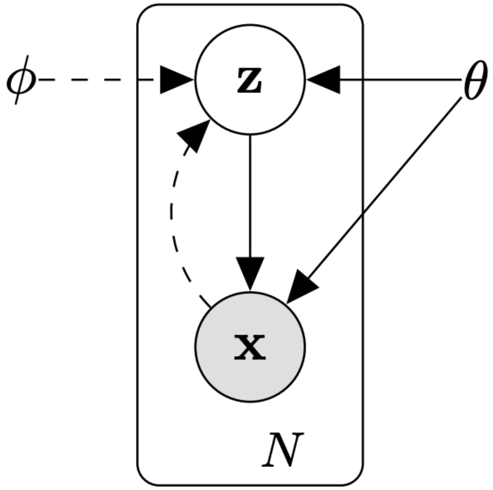
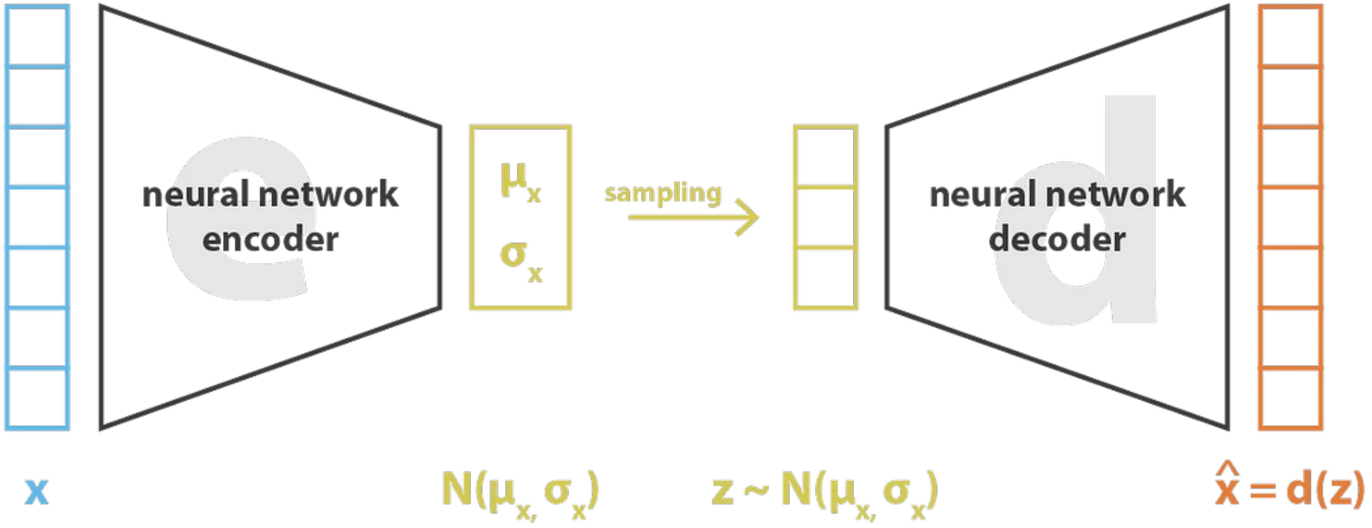


Illustration of VAEs:



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

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Image Credit: [6]

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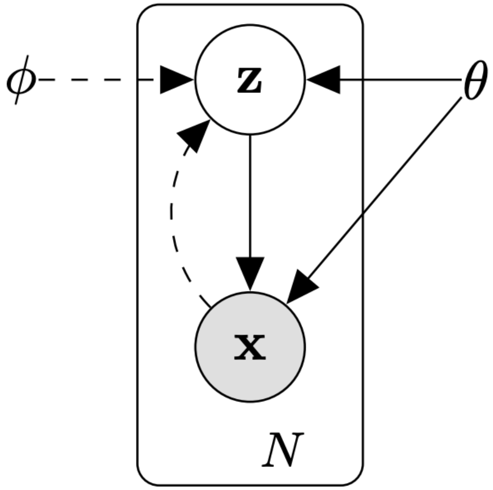
  - Reparameterization Trick
- Graph Variational Autoencoders

Amortized Variational Inference



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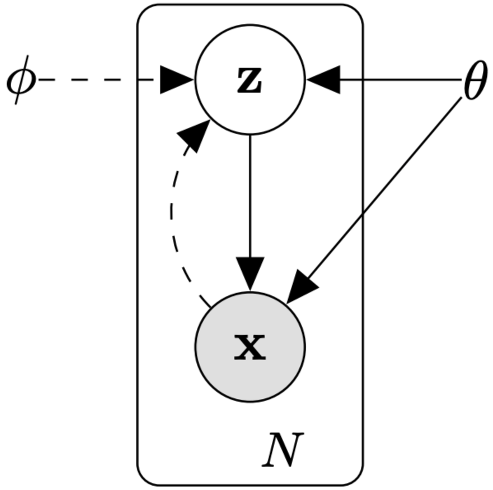
Encoder is amortized: every X shares the same set of parameters ϕ

Amortized Variational Inference



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

$$
\begin{aligned}
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\end{aligned}
$$

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

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

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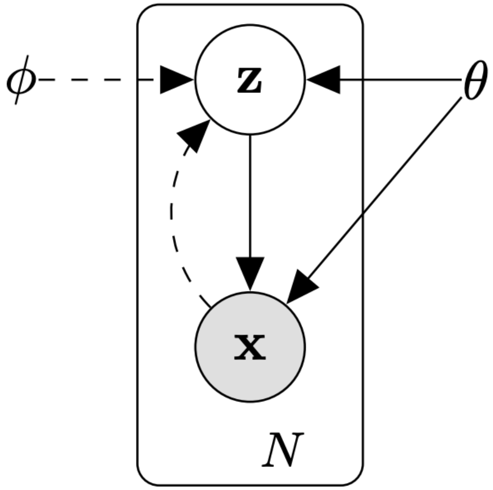
We thus only need to optimize ELBO over one set of parameters ϕ, whereas in traditional variational inference (VI) one needs to find the optimal variational distribution per X

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

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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]:

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

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

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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&= \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,

$$q_\phi(Z|X) = \mathcal{N}(Z|\mu_\phi(X), \sigma_\phi(X)^2 I)$$
$$p_\theta(Z) = \mathcal{N}(X|0, I)$$

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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

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

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

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

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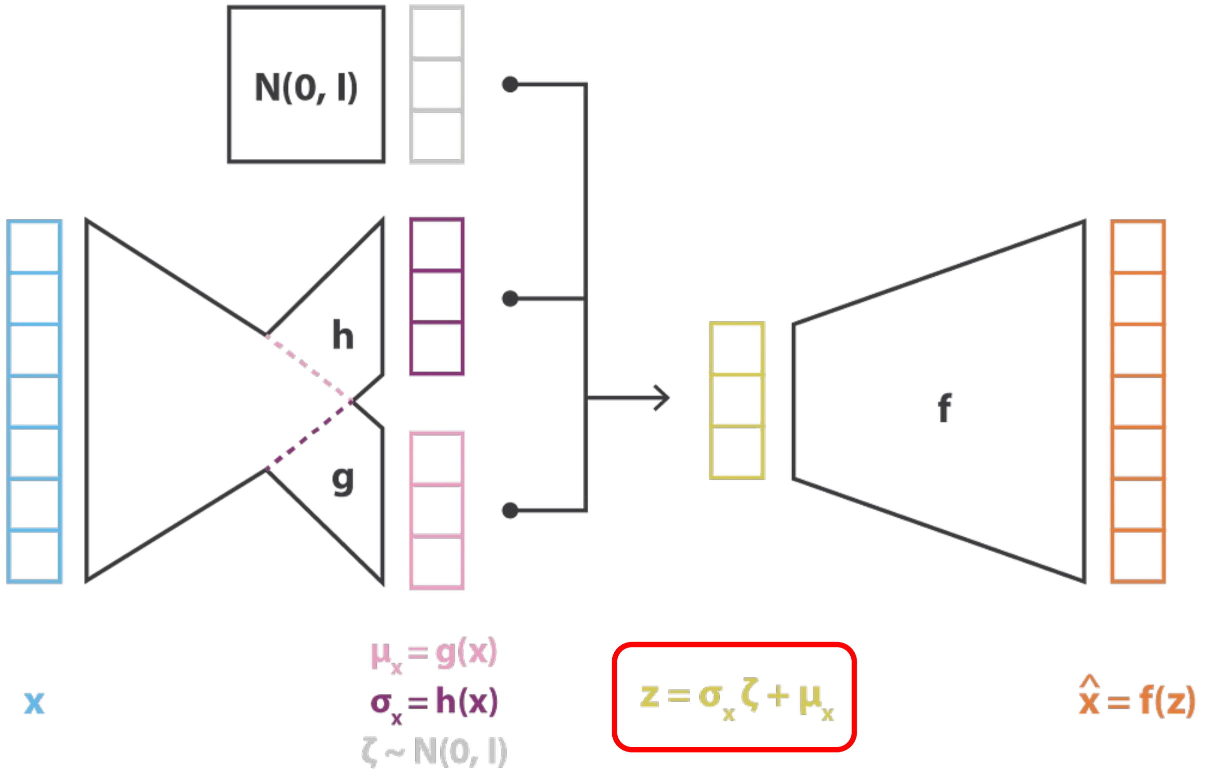
\end{aligned}
$$

Now we can get the gradient directly!

Reparameterization Trick

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



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

Image Credit: [6]

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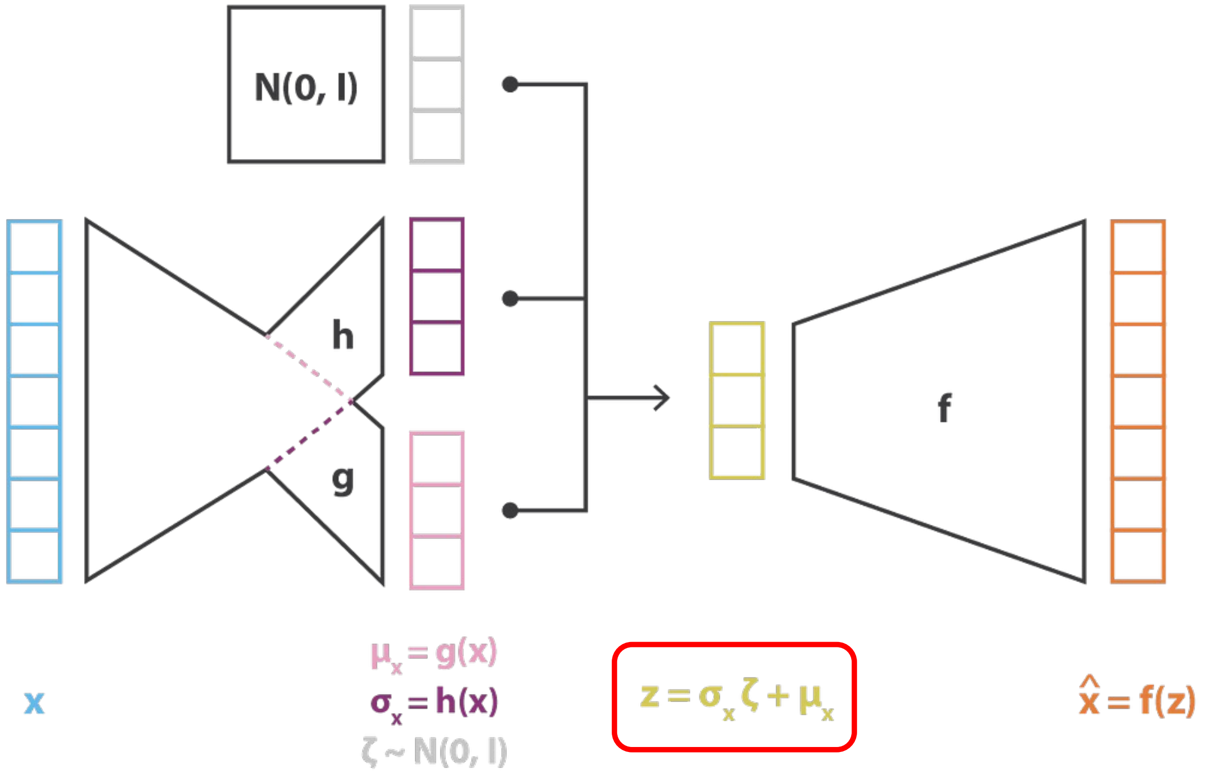

$$\text{loss} = C \, || x - \hat{x} ||^2 + KL[\, N(\mu_x, \sigma_x), N(0, I) \,] = C \, || x - f(z) ||^2 + KL[\, N(g(x), h(x)), N(0, I) \,]$$

What if we have discrete latent variables in VAEs?

Image Credit: [6]

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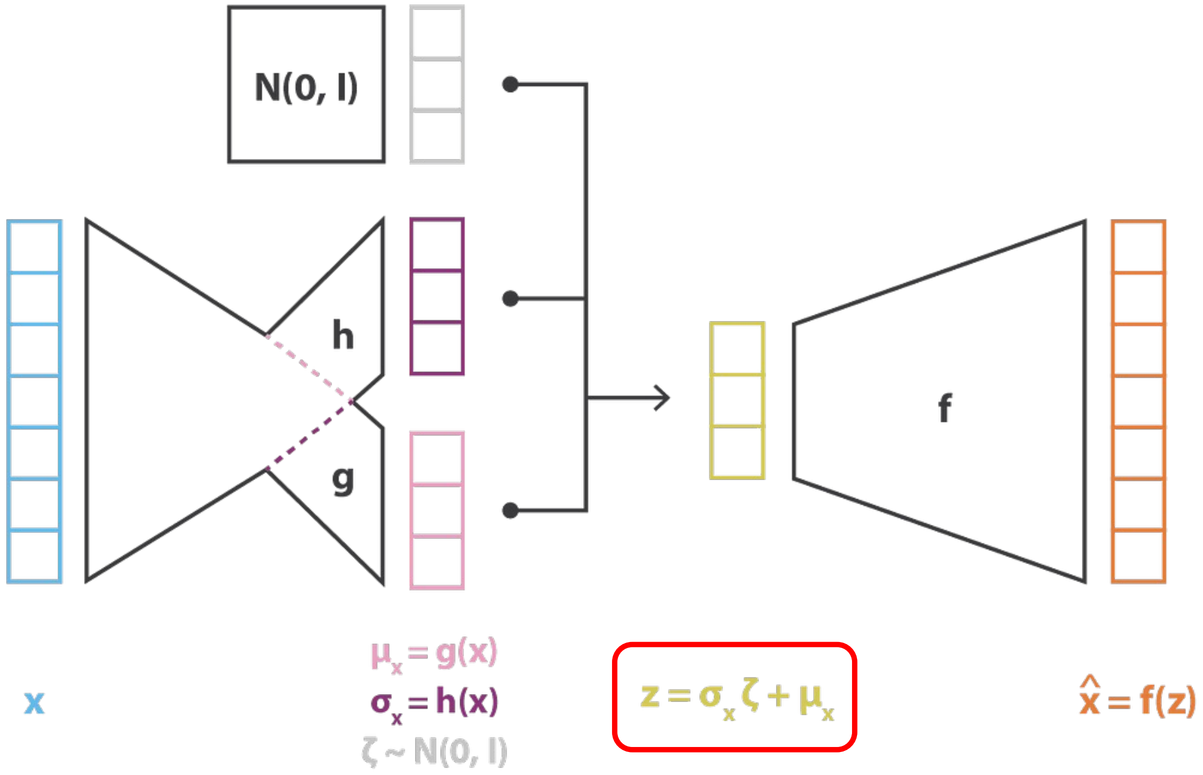
In the illustration of VAEs, the latent variable is *reparameterized* as below:



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

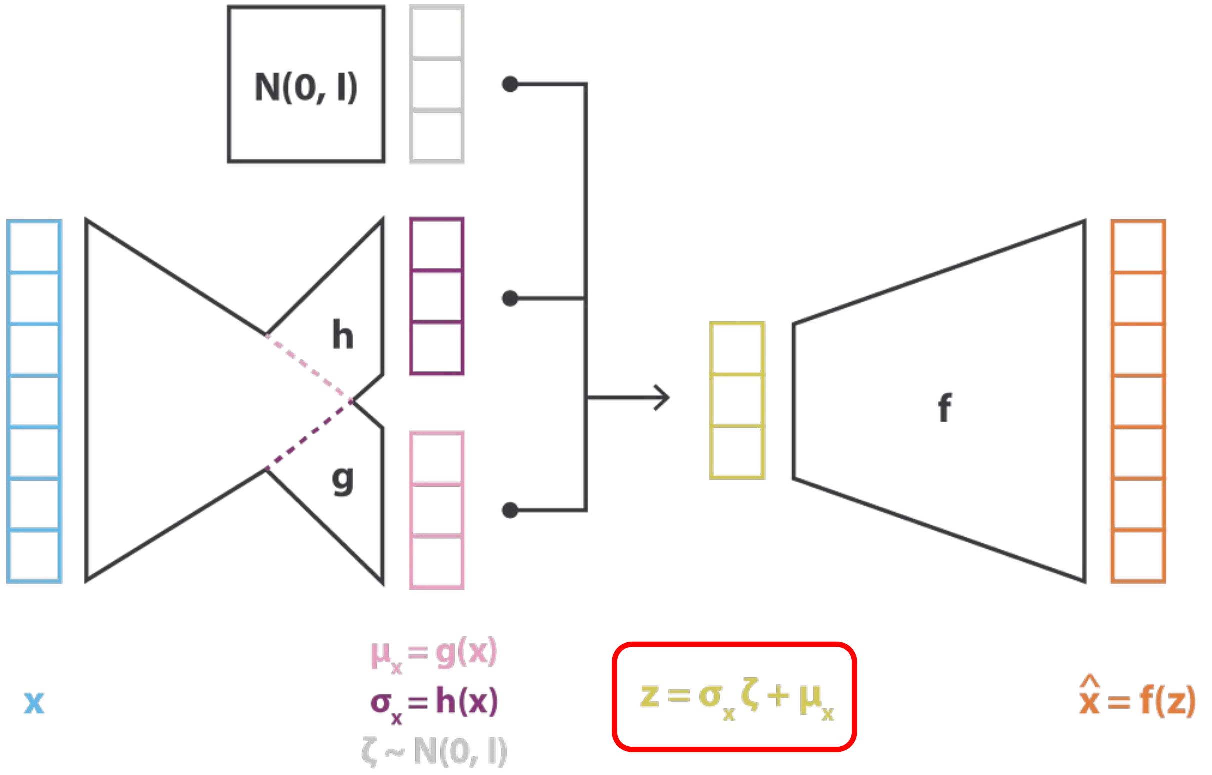
What if we have discrete latent variables in VAEs?

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

Image Credit: [6]

Reparameterization Trick

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?

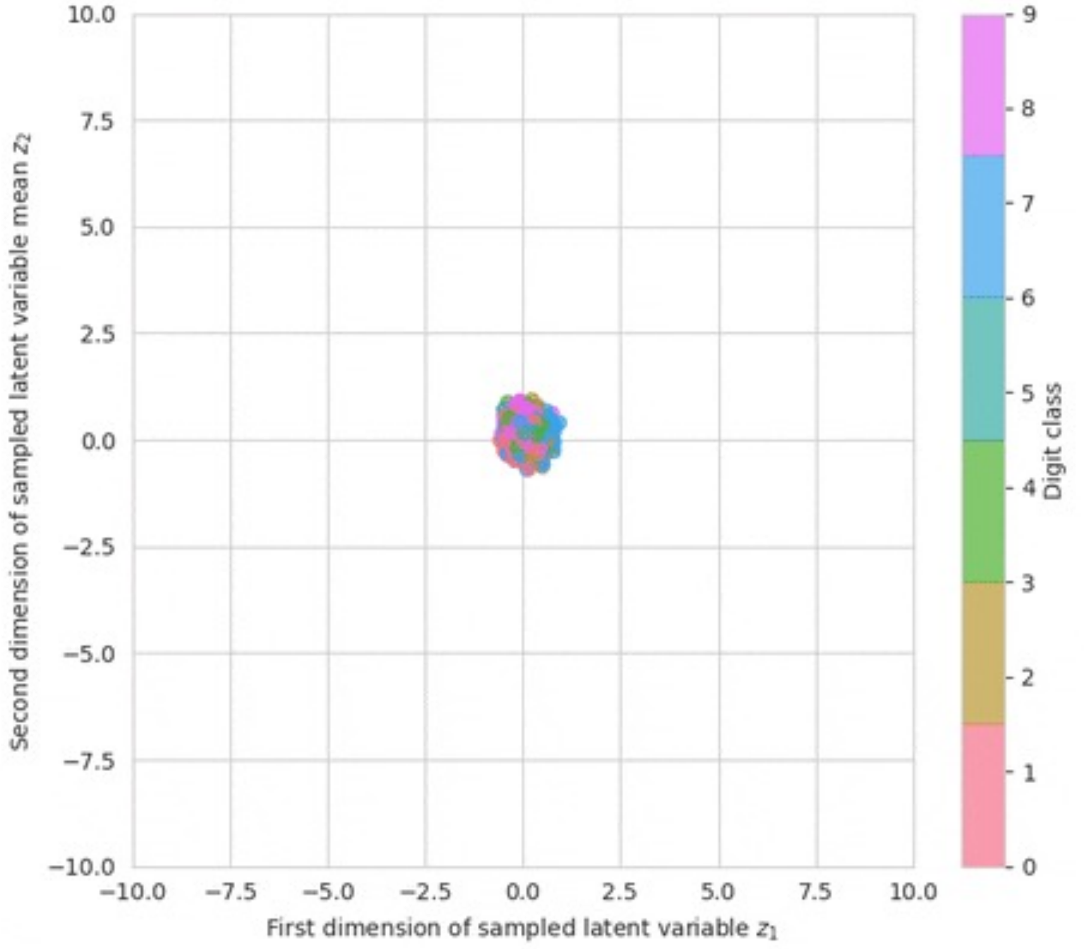
Reparameterization trick does not work exactly since sampling path is non-differentiable!

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:

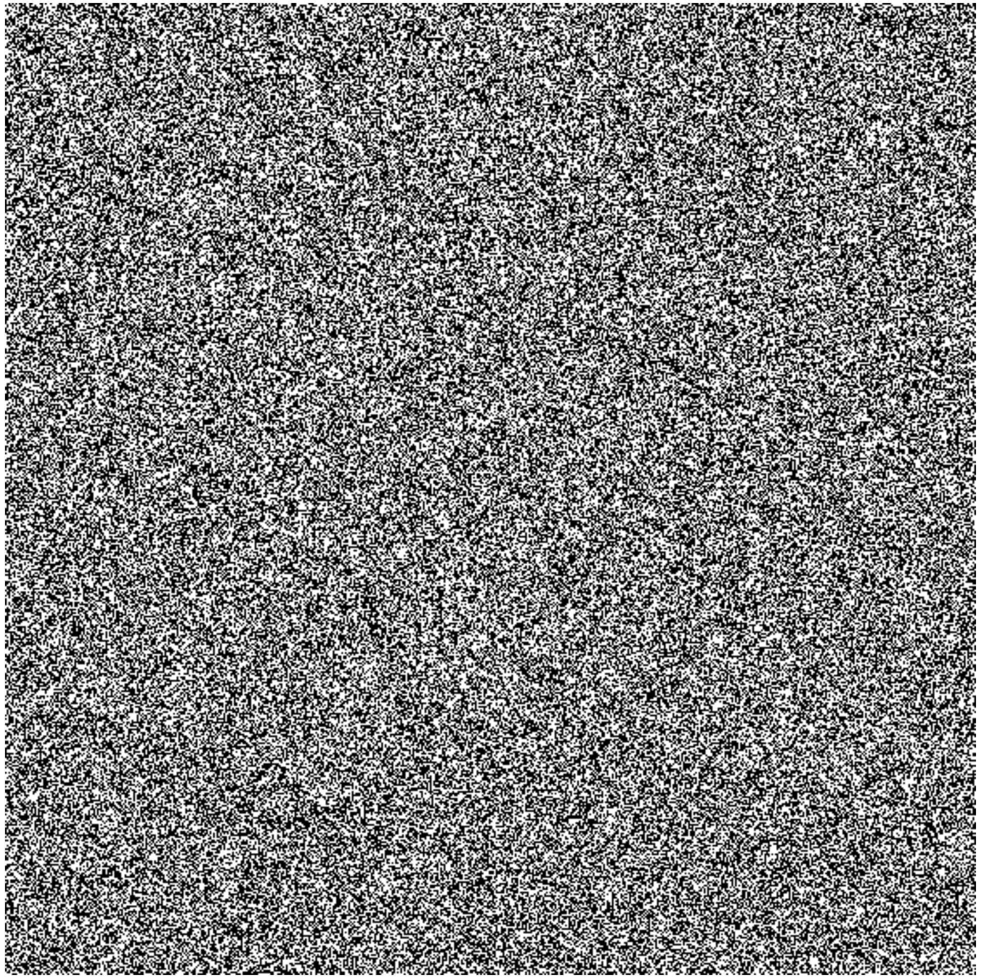


Image Credit: [9]

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:

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

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\mu_i, \log\sigma_i^2 &= \mathrm{Readout}_\phi(H)
\end{aligned}
$$

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

Graph VAEs [10, 11]:

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

Adjacency Matrix Decoder:
$$p_\theta(A|Z) = \prod_i \prod_j p_\theta(A_{ij}|Z)$$
$$H = \mathrm{MLP}(Z)$$
$$p_\theta(A_{ij} = 1|Z_i, Z_j) = \sigma(H_i^\top H_j)$$

Graph Variation Autoencoders

Graph VAEs [10, 11]:

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

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

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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\log p_\theta(X, A) &\geq \text{ELBO} \\
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\end{aligned}
$$

Are we done?

No! We hope ELBO is permutation invariant!

Graph Variation Autoencoders

Graph VAEs [10, 11]:

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$$
\begin{aligned}
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\end{aligned}
$$

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) \\
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Graph Variation Autoencoders

Graph VAEs [10, 11]:

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

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

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:

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

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

Graph VAEs [10, 11]:

Learning:

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

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)

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

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Questions?