VAE

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Laboratory for methods of big data analysis

LAMBDA • HSE

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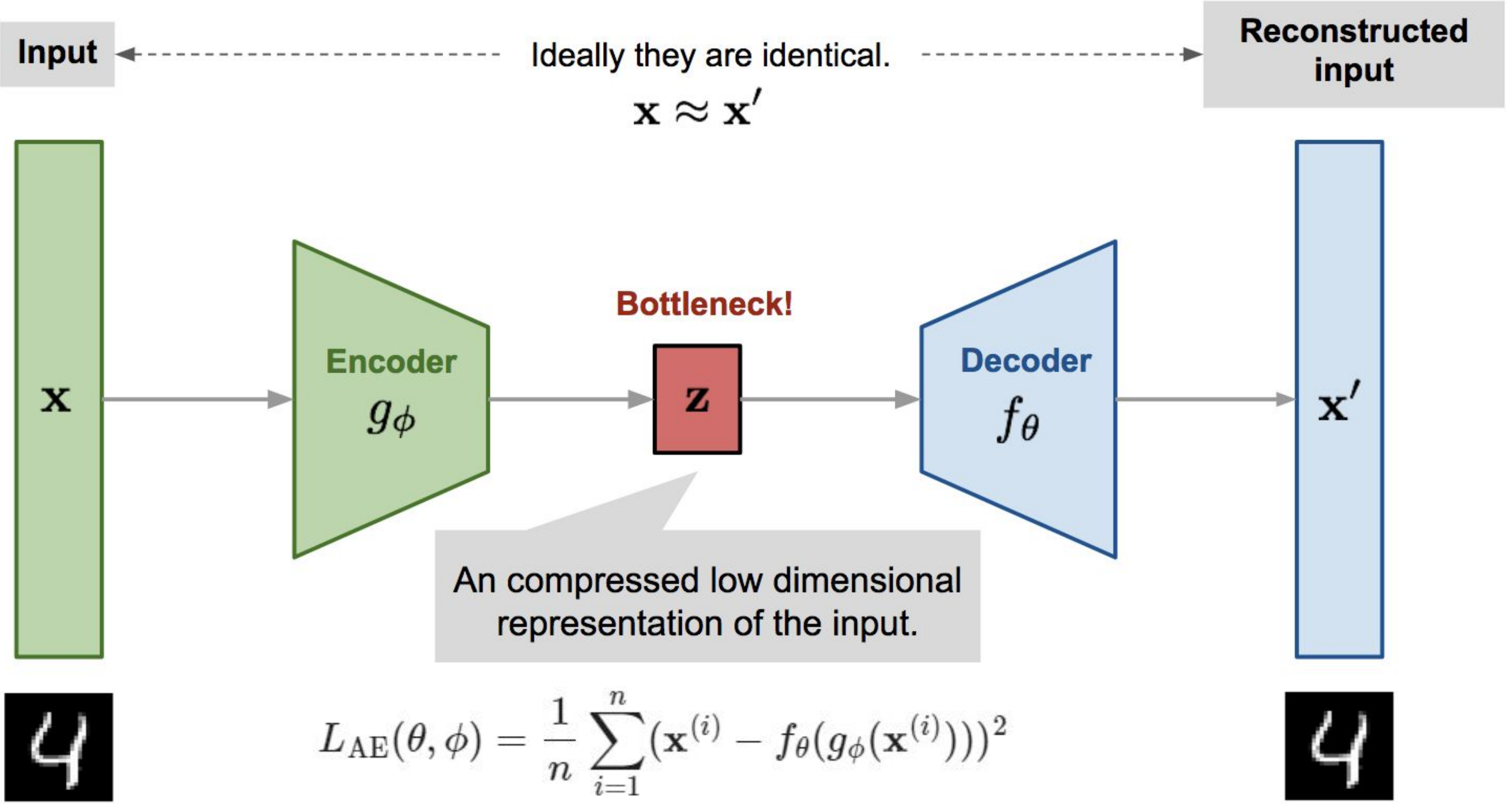
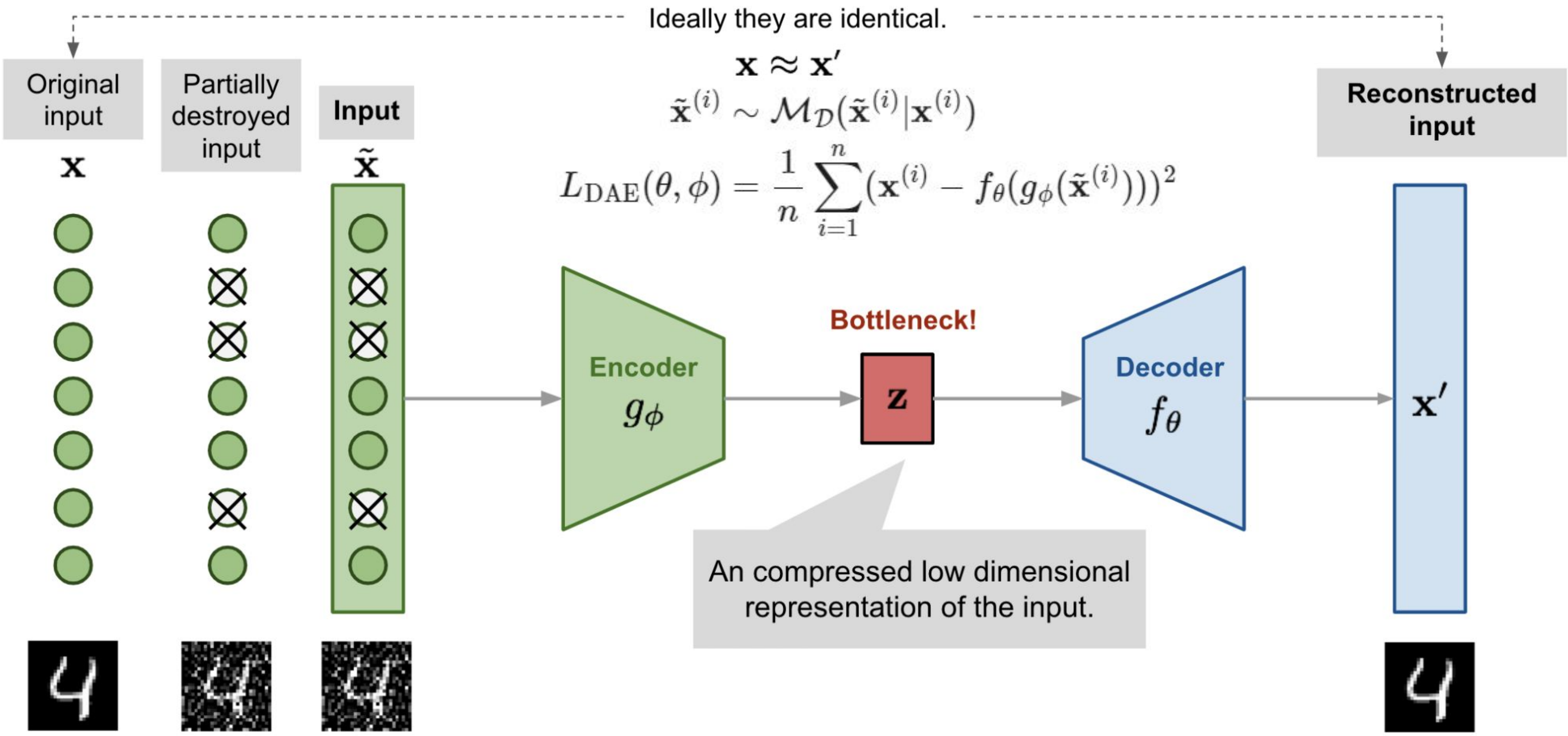
Autoencoders

Idea


Input
Ideally they are identical.
$\mathbf{x} \approx \mathbf{x}'$
Reconstructed input
$\mathbf{x}$
Encoder
g_ϕ
Bottleneck!
$\mathbf{z}$
Decoder
f_θ
$\mathbf{x}'$
An compressed low dimensional representation of the input.
$$L_{\mathrm{AE}}(\theta, \phi) = \frac{1}{n} \sum_{i=1}^{n} (\mathbf{x}^{(i)} - f_\theta(g_\phi(\mathbf{x}^{(i)})))^2$$

Denoising AE



VAE

VAE

- Instead of mapping the input into a *fixed* vector z, we want to map it into distribution p_θ parameterized by θ
- In this setup, the relation between the input data x and the latent encoding vector z can be defined in terms of bayesian framework.
- Prior $p_\theta(\mathrm{z})$
- Likelihood $p_\theta(\mathrm{x}|\mathrm{z})$
- Posterior $p_\theta(\mathrm{z}|\mathrm{x})$

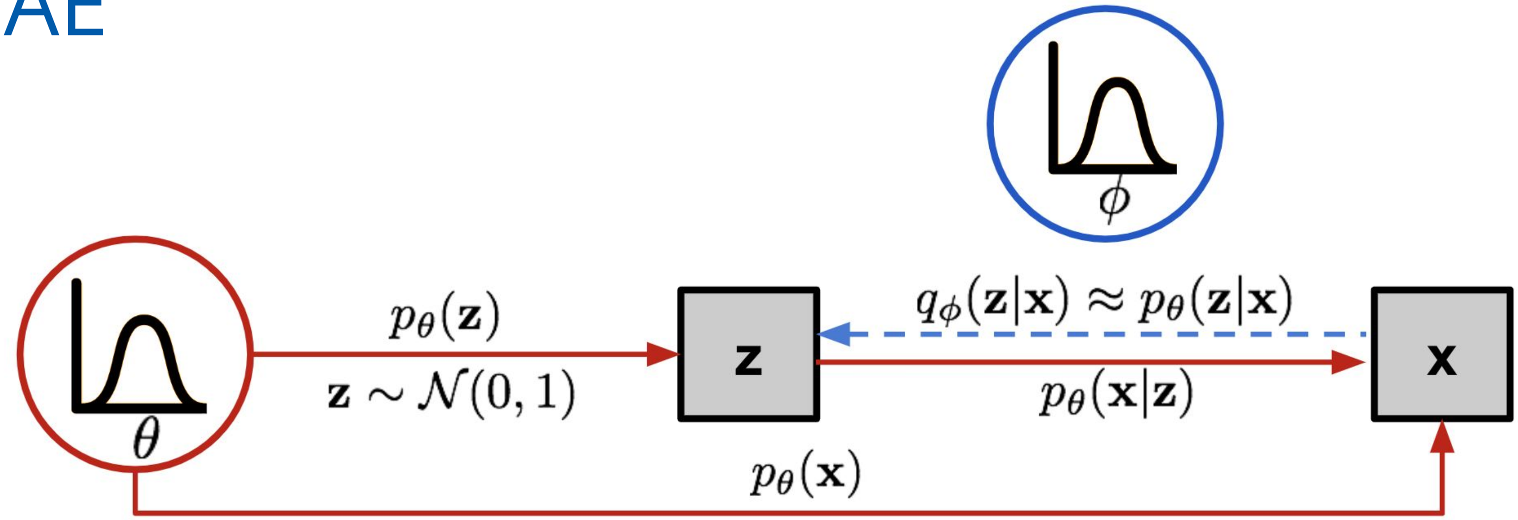
VAE

- Assume we know θ^*
- First, sample a $\mathbf{z}^{(\mathbf{i})}$ from a prior distribution $p_\theta(z)$
- Then a value $\mathbf{x}^{(\mathbf{i})}$ is generated from a conditional distribution $p_\theta(x|z=z^{(i)})$
- Optimality:

$$\theta^* = \arg\max_\theta \prod_{i=1}^{n} p_\theta(\mathbf{x}^{(i)}) \qquad \theta^* = \arg\max_\theta \sum_{i=1}^{n} \log p_\theta(\mathbf{x}^{(i)})$$

$$p_\theta(\mathbf{x}^{(i)}) = \int p_\theta(\mathbf{x}^{(i)}|\mathbf{z}) p_\theta(\mathbf{z}) d\mathbf{z}$$

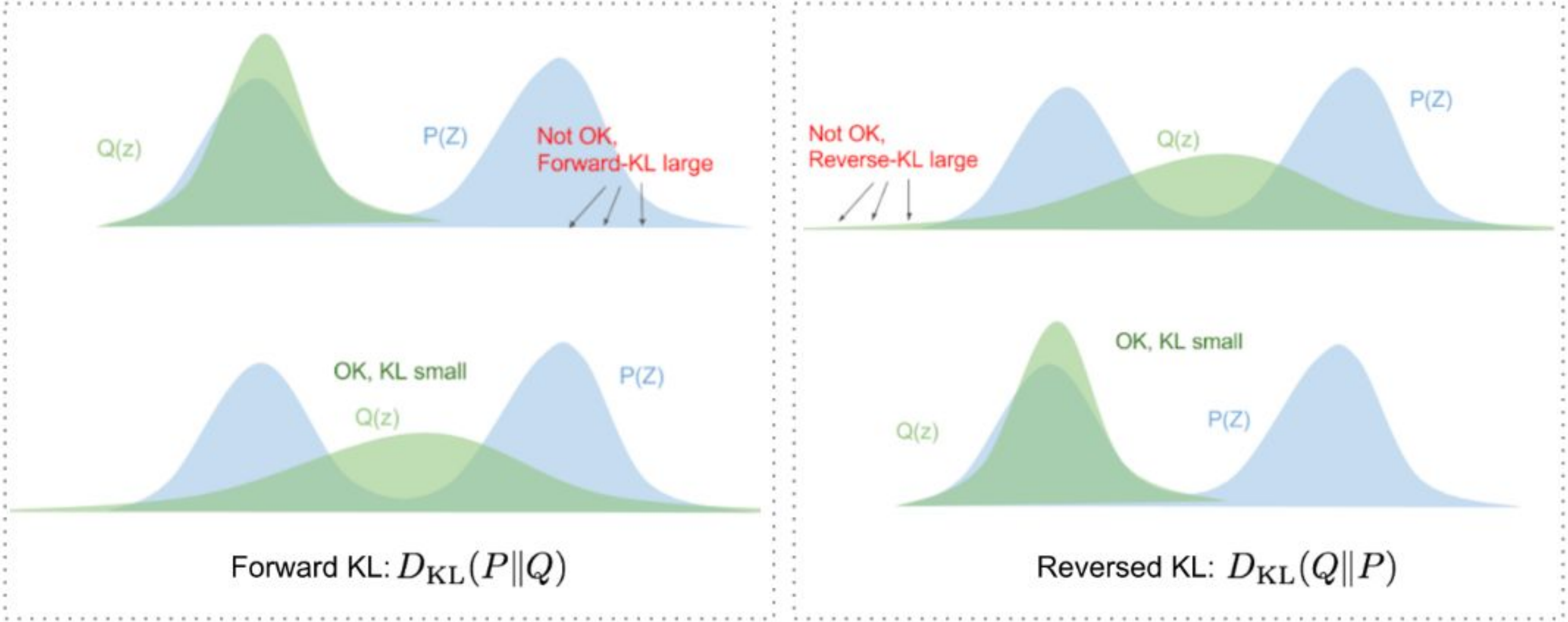
VAE



- It is not easy to compute, since it is very expensive to check all the possible values of z
- Thus, let's introduce a new approximation function $q_\varphi(z|x)$
- Now, the structure looks a lot like AE, where conditional probability $p_\theta(x|z)$ defines a generative models, similar to decoder, and it is also called *probabilistic decoder*, and the approximation function $q_\varphi(z|x)$ is the *probabilistic encoder*.

ELBO

ELBO



- The estimated posterior $q_{\varphi}(z|x)$ should be very close the real one $p_{\theta}(x|z)$
- We can use KL divergence $D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})|p_\theta(\mathbf{z}|\mathbf{x}))$

ELBO

$$
\begin{aligned}
&D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z}|\mathbf{x})) \\
&= \int q_\phi(\mathbf{z}|\mathbf{x}) \log \frac{q_\phi(\mathbf{z}|\mathbf{x})}{p_\theta(\mathbf{z}|\mathbf{x})} d\mathbf{z} \\
&= \int q_\phi(\mathbf{z}|\mathbf{x}) \log \frac{q_\phi(\mathbf{z}|\mathbf{x})p_\theta(\mathbf{x})}{p_\theta(\mathbf{z},\mathbf{x})} d\mathbf{z} && \text{; Because } p(z|x)=p(z,x)/p(x) \\
&= \int q_\phi(\mathbf{z}|\mathbf{x}) \big(\log p_\theta(\mathbf{x}) + \log \frac{q_\phi(\mathbf{z}|\mathbf{x})}{p_\theta(\mathbf{z},\mathbf{x})} \big) d\mathbf{z} \\
&= \log p_\theta(\mathbf{x}) + \int q_\phi(\mathbf{z}|\mathbf{x}) \log \frac{q_\phi(\mathbf{z}|\mathbf{x})}{p_\theta(\mathbf{z},\mathbf{x})} d\mathbf{z} && \text{; Because } \textstyle\int q(z|x)dz=1 \\
&= \log p_\theta(\mathbf{x}) + \int q_\phi(\mathbf{z}|\mathbf{x}) \log \frac{q_\phi(\mathbf{z}|\mathbf{x})}{p_\theta(\mathbf{x}|\mathbf{z})p_\theta(\mathbf{z})} d\mathbf{z} && \text{; Because } p(z,x)=p(x|z)p(z) \\
&= \log p_\theta(\mathbf{x}) + \mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})}[\log \frac{q_\phi(\mathbf{z}|\mathbf{x})}{p_\theta(\mathbf{z})} - \log p_\theta(\mathbf{x}|\mathbf{z})] \\
&= \log p_\theta(\mathbf{x}) + D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z})) - \mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})} \log p_\theta(\mathbf{x}|\mathbf{z})
\end{aligned}
$$

ELBO

$$D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z}|\mathbf{x})) = \log p_\theta(\mathbf{x}) + D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z})) - \mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})}\log p_\theta(\mathbf{x}|\mathbf{z})$$

$$\log p_\theta(\mathbf{x}) - D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z}|\mathbf{x})) = \mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})}\log p_\theta(\mathbf{x}|\mathbf{z}) - D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z}))$$

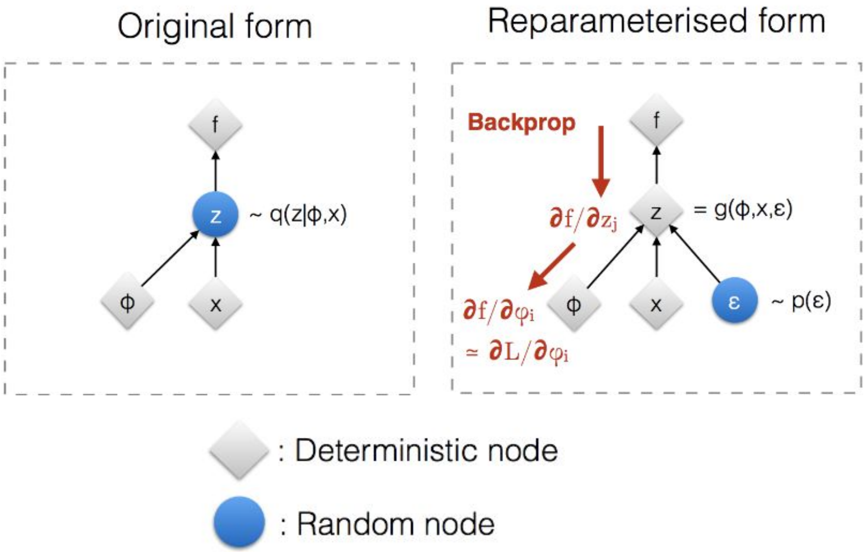
$$\begin{aligned} L_{\mathrm{VAE}}(\theta,\phi) &= -\log p_\theta(\mathbf{x}) + D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z}|\mathbf{x})) \\ &= -\mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})}\log p_\theta(\mathbf{x}|\mathbf{z}) + D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z})) \\ \theta^*, \phi^* &= \arg\min_{\theta,\phi} L_{\mathrm{VAE}} \end{aligned}$$

Since KL divergence is always non-negative and thus $-L_{\mathrm{VAE}}$ is the lower bound of $\log p_\theta(x)$

$$-L_{\mathrm{VAE}} = \log p_\theta(\mathbf{x}) - D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z}|\mathbf{x})) \leq \log p_\theta(\mathbf{x})$$

Reparametrization trick

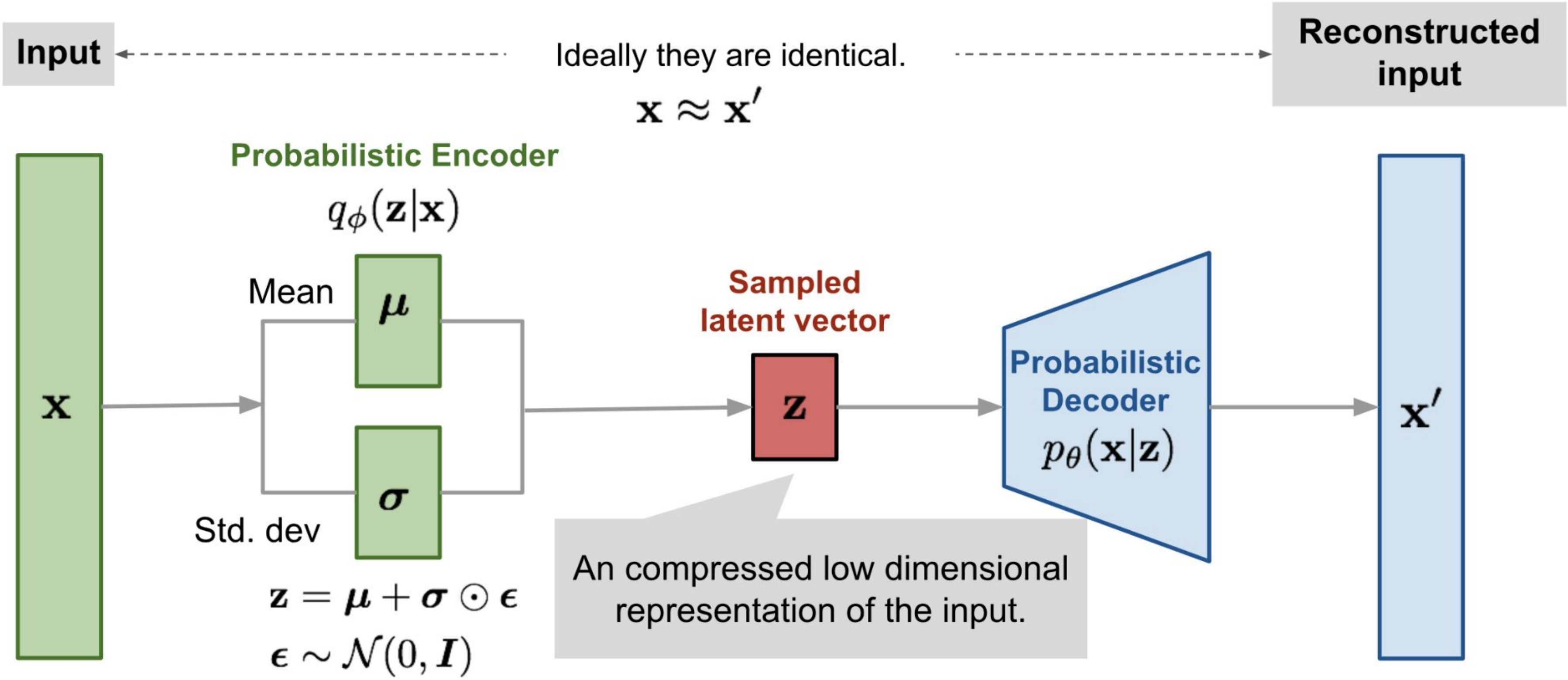
- The expectation term in the loss function invokes generating samples from $z \sim q_\varphi(z|x)$
- Sampling is a stochastic process, and cannot be backpropagated
- Thus, let's introduce the reparametrization trick:



$$\mathbf{z} \sim q_\phi(\mathbf{z}|\mathbf{x}^{(i)}) = \mathcal{N}(\mathbf{z}; \boldsymbol{\mu}^{(i)}, \boldsymbol{\sigma}^{2(i)}\boldsymbol{I})$$

$$\mathbf{z} = \boldsymbol{\mu} + \boldsymbol{\sigma} \odot \boldsymbol{\epsilon}, \text{ where } \boldsymbol{\epsilon} \sim \mathcal{N}(0, \boldsymbol{I}) \qquad \text{; Reparameterization trick.}$$

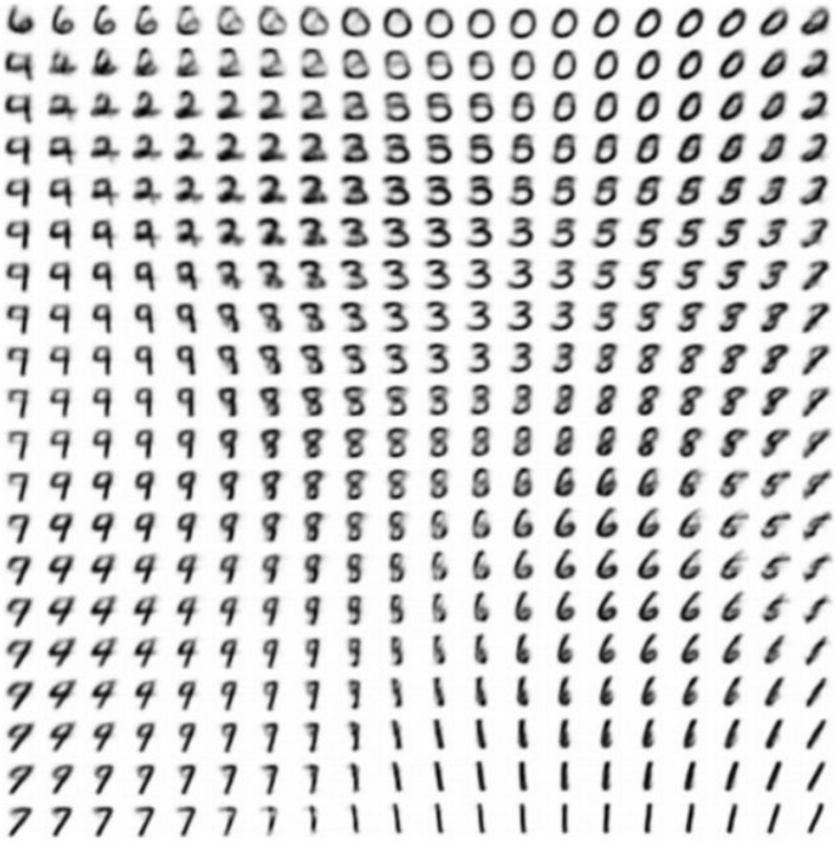
VAE



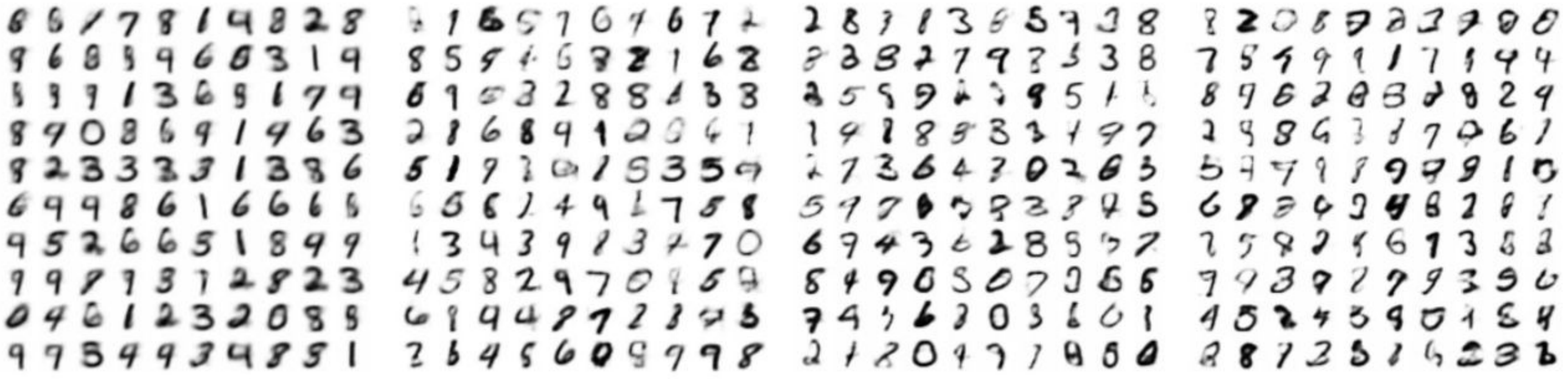
Input
Ideally they are identical.
$\mathbf{x} \approx \mathbf{x}'$
Reconstructed input
Probabilistic Encoder
$q_\phi(\mathbf{z}|\mathbf{x})$
Mean
$\boldsymbol{\mu}$
Std. dev
$\boldsymbol{\sigma}$
$\mathbf{x}$
Sampled latent vector
$\mathbf{z}$
Probabilistic Decoder
$p_\theta(\mathbf{x}|\mathbf{z})$
$\mathbf{x}'$
$\mathbf{z} = \boldsymbol{\mu} + \boldsymbol{\sigma} \odot \boldsymbol{\epsilon}$
$\boldsymbol{\epsilon} \sim \mathcal{N}(0, \boldsymbol{I})$
An compressed low dimensional representation of the input.

Results

- The latent space is well organized
- The results does not suffer from mode collapse
- The sampling speed is decent
- Images are blurred



Results



(a) 2-D latent space (b) 5-D latent space (c) 10-D latent space (d) 20-D latent space

Results

Due to minimization of KL

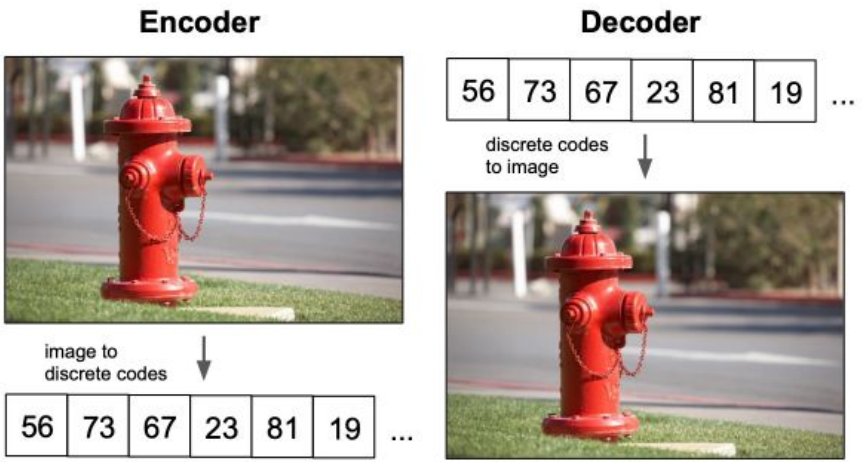
$$KL\big(q(z;\phi)\big|\big|p(z|x;\theta)\big) \to 0.$$

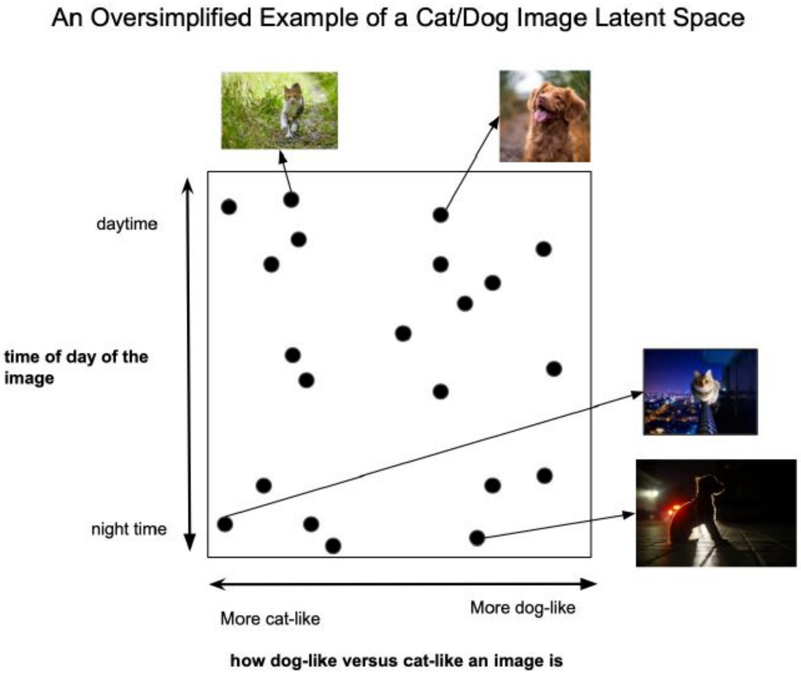
VQ-VAE

Latemd Spaces

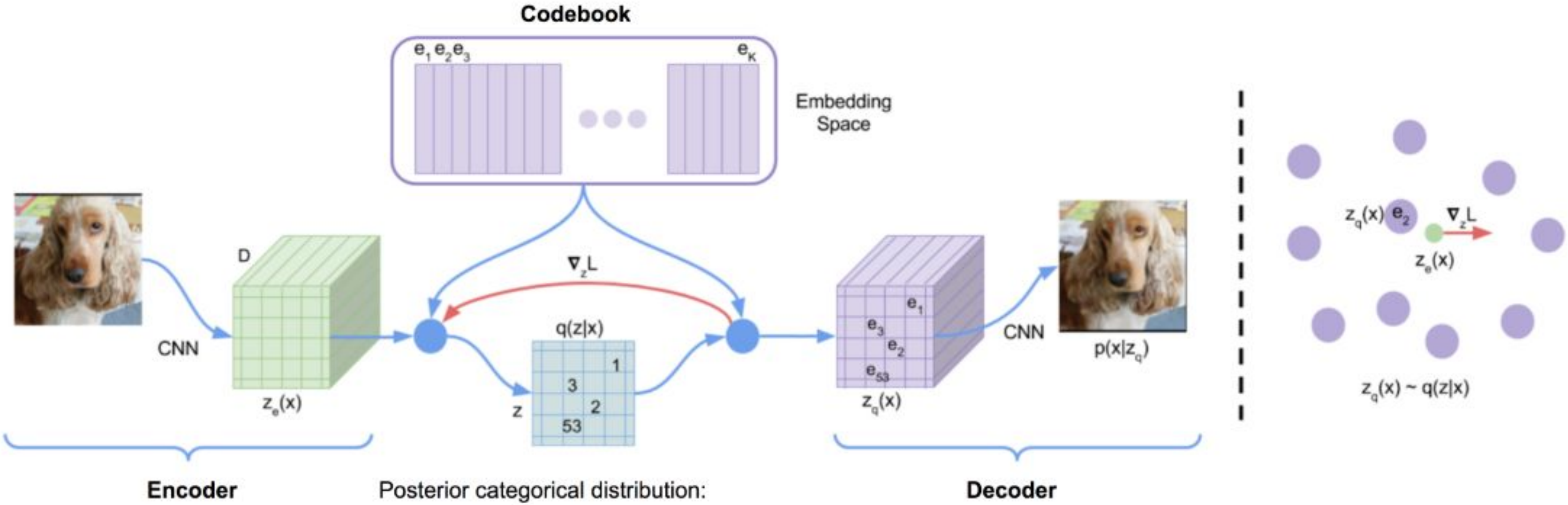
VAE gives a good representations

Can we study it?





VQ-VAE



$$q(\mathbf{z}=\mathbf{e}_k|\mathbf{x}) = \begin{cases} 1 & \text{if } k = \arg\min_i \|\mathbf{z}_e(\mathbf{x}) - \mathbf{e}_i\|_2 \\ 0 & \text{otherwise.} \end{cases}$$

$$L = \underbrace{\|\mathbf{x} - D(\mathbf{e}_k)\|_2^2}_{\text{reconstruction loss}} + \underbrace{\|\text{sg}[E(\mathbf{x})] - \mathbf{e}_k\|_2^2}_{\text{VQ loss}} + \underbrace{\beta\|E(\mathbf{x}) - \text{sg}[\mathbf{e}_k]\|_2^2}_{\text{commitment loss}}$$