भारतीय प्रौद्योगिकी संस्थान दिल्ली
Indian Institute of Technology Delhi

COV877
Special Module on Visual Computing

Generative AI for Visual Content Creation: Image, Video, and 3D

VAE & VQVAE

Instructor:

Dr. Lokender Tiwari

Research Scientist

Variational Autoencoder (VAE)

Variational Autoencoders

- Probabilistic Generative Model (like normalizing flows)
- Learn distribution $Pr(\mathbf{x})$ over data
- Post training we can sample from this distribution

Latent Variable Model

- An indirect approach to represent probability distribution of data $Pr(\mathbf{x})$

$$Pr(\mathbf{x}) = \underbrace{\int \overbrace{\boxed{Pr(\mathbf{x}, \mathbf{z})}}^{\text{joint distribution of data \& unobserved latent variable}} d\mathbf{z}}_{\text{marginalization}}$$

conditional probability

$$Pr(\mathbf{x}) = \int \underbrace{Pr(\mathbf{x}|\mathbf{z})}_{\text{likelihood}} \overbrace{Pr(\mathbf{z})}^{\text{prior}} d\mathbf{z}$$

complex distributions $Pr(\mathbf{x})$ can be represented using simple $Pr(\mathbf{x}|\mathbf{z})$ and $Pr(\boldsymbol{z})$

e.g. Mixture of Gaussians

Latent Variable Model - Mixture of Gaussian Example

- $\mathbf{z}$ is a discrete latent variable with categorial prior distribution $Pr(\mathbf{z})$

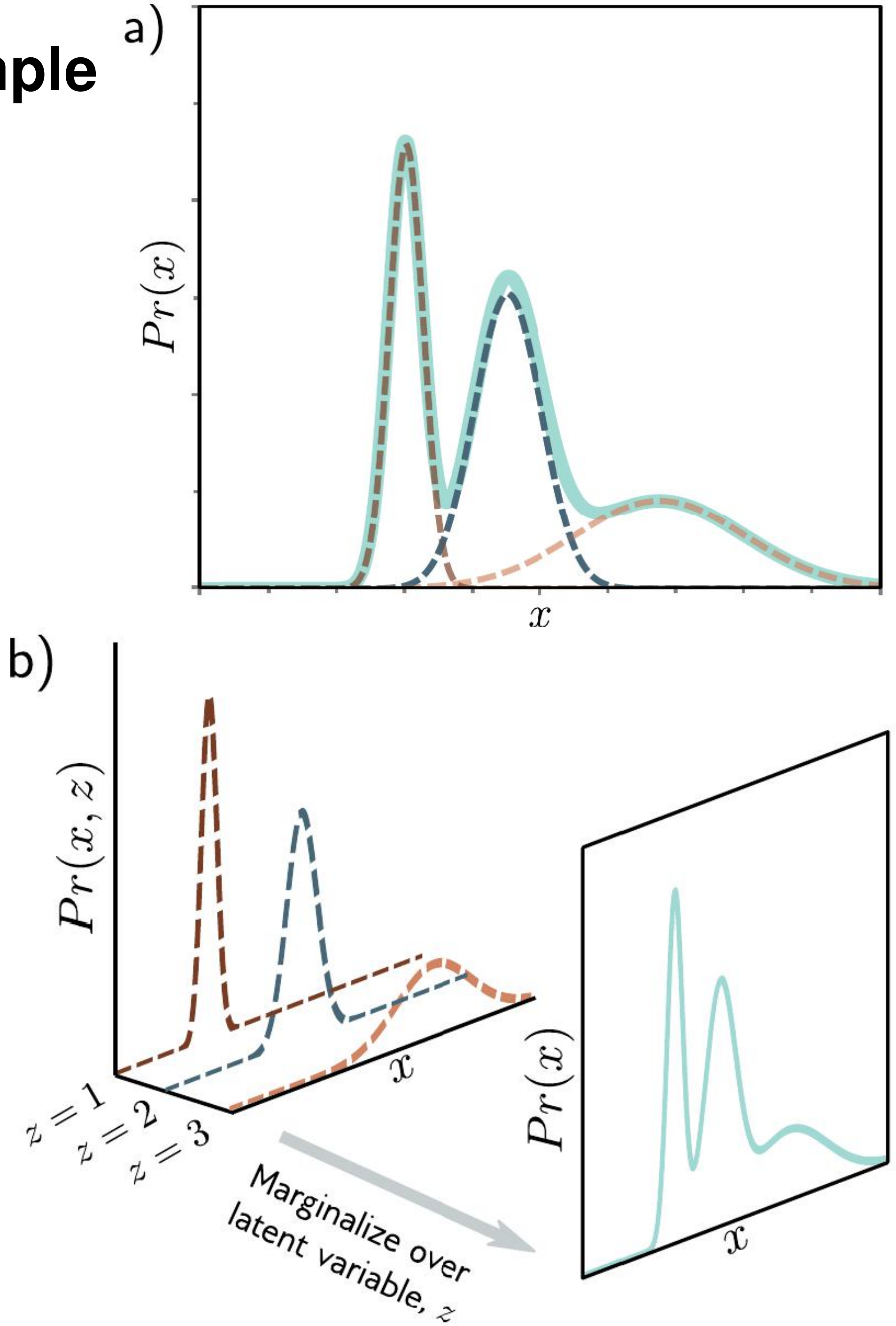
$$Pr(z=n) \quad = \quad \lambda_n$$

- Likelihood $Pr(\mathbf{x}|\mathbf{z}=\mathbf{n})$ of data $\mathbf{x}$ given $\mathbf{z}=\mathbf{n}$ is normally distributed with mean μ_n and variance σ_n^2

$$Pr(x|z=n) \quad = \quad \text{Norm}_x\left[\mu_n, \sigma_n^2\right]$$

$$\begin{aligned} Pr(x) &= \sum_{n=1}^{N} Pr(x, z=n) \\ &= \sum_{n=1}^{N} Pr(x|z=n) \cdot Pr(z=n) \\ &= \sum_{n=1}^{N} \lambda_n \cdot \text{Norm}_x\left[\mu_n, \sigma_n^2\right]. \end{aligned}$$

Marginalization



Nonlinear Latent Variable Model

Both data $\mathbf{x}$ and latent variable $\mathbf{z}$ are continous and multivariate

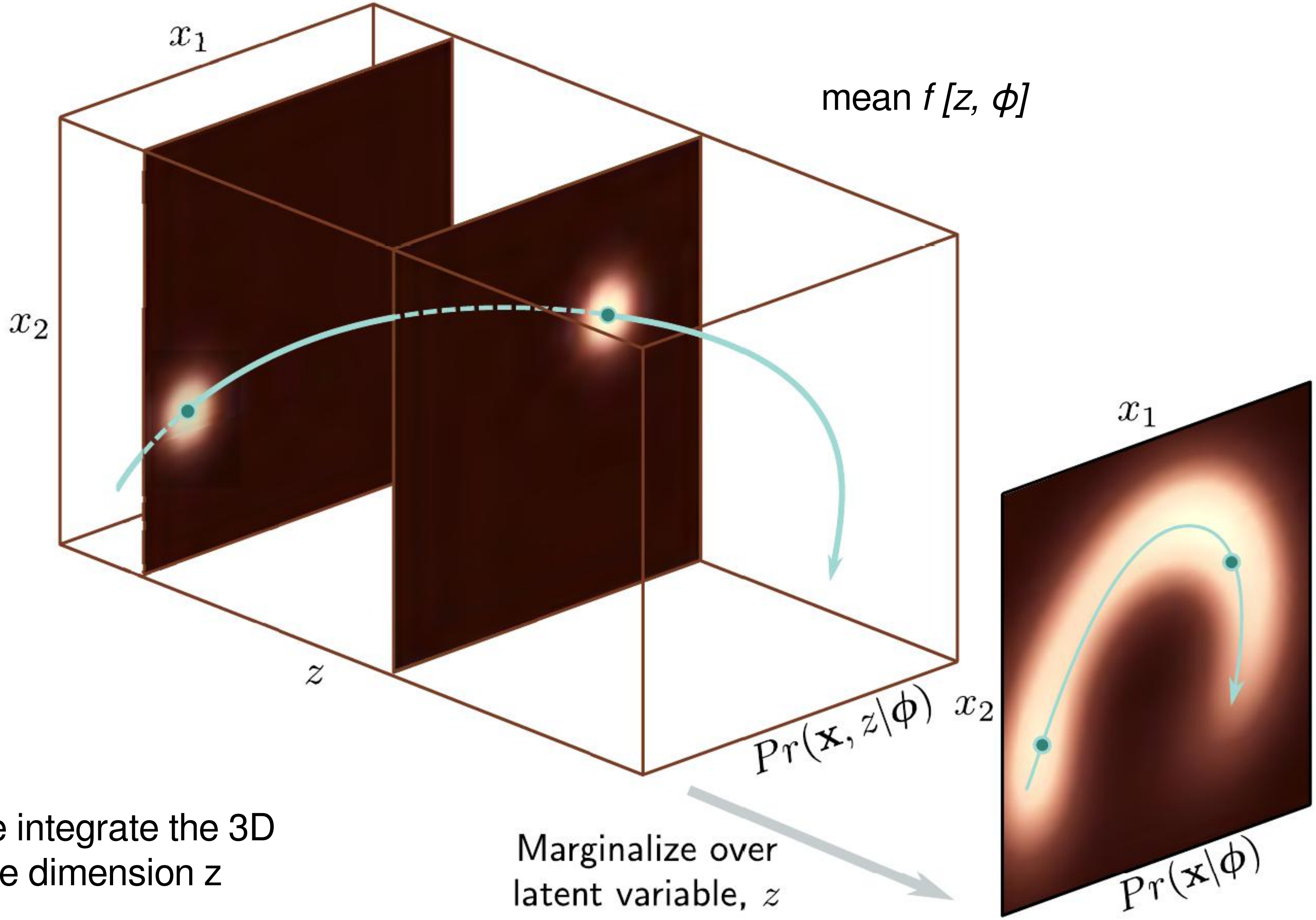
$$Pr(\mathbf{z}) = \text{Norm}_{\mathbf{z}}[\mathbf{0}, \mathbf{I}]$$

likelihood $$Pr(\mathbf{x}|\mathbf{z}, \phi) = \text{Norm}_{\mathbf{x}}\left[\mathbf{f}[\mathbf{z}, \phi], \sigma^2\mathbf{I}\right]$$ mean is a nonlinear function of the latent variable

$$\begin{aligned}
Pr(\mathbf{x}|\phi) &= \int Pr(\mathbf{x}, \mathbf{z}|\phi) d\mathbf{z} \\
&= \int Pr(\mathbf{x}|\mathbf{z}, \phi) \cdot Pr(\mathbf{z}) d\mathbf{z} \\
&= \int \text{Norm}_{\mathbf{x}}\left[\mathbf{f}[\mathbf{z}, \phi], \sigma^2\mathbf{I}\right] \cdot \text{Norm}_{\mathbf{z}}\left[\mathbf{0}, \mathbf{I}\right] d\mathbf{z}
\end{aligned}$$

Nonlinear Latent Variable Model

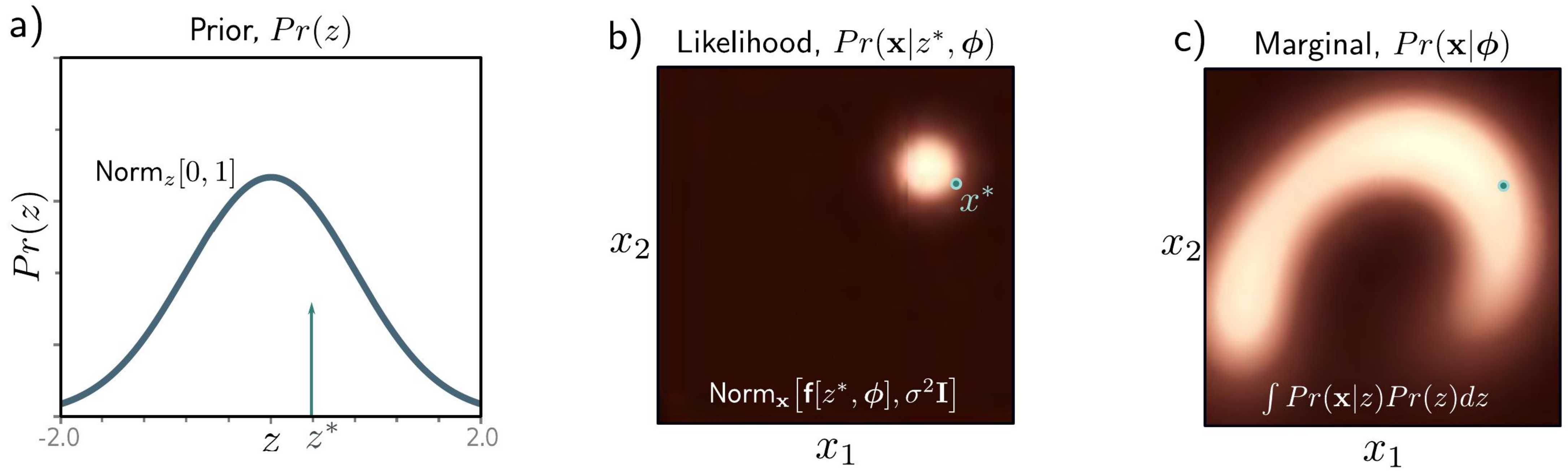
- Both data $\mathbf{x}$ and latent variable $\mathbf{z}$ are continous and multivariate



to get $Pr(x)$, we integrate the 3D volume over the dimension z

Nonlinear Latent Variable Model - Generation from nonlinear latent variable model

- Both data $\mathbf{x}$ and latent variable $\mathbf{z}$ are continous and multivariate



Nonlinear Latent Variable Model - Training

- Maximize the log-likelihood w.r.t the model parameters over training set

- For simplicity assume the variance term is known

- Goal is to learn Φ

$$\hat{\boldsymbol{\phi}} = \underset{\boldsymbol{\phi}}{\operatorname{argmax}} \left[\sum_{i=1}^{I} \log \left[Pr(\mathbf{x}_i | \boldsymbol{\phi}) \right] \right]$$

$$Pr(\mathbf{x}_i | \boldsymbol{\phi}) = \int \operatorname{Norm}_{\mathbf{x}_i} [\mathbf{f}[\mathbf{z}, \boldsymbol{\phi}], \sigma^2 \mathbf{I}] \cdot \operatorname{Norm}_{\mathbf{z}} [\mathbf{0}, \mathbf{I}] d\mathbf{z}$$

- Unfortunately, this is intractable.
- There is no closed-form expression for the integral and no easy way to evaluate it for a particular value of x

Nonlinear Latent Variable Model - ELBO

$$\hat{\phi} = \underset{\phi}{\operatorname{argmax}} \left[\sum_{i=1}^{I} \log\left[Pr(\mathbf{x}_i|\phi) \right] \right]$$

- Define lower bound on the log-likelihood
- a function which is always less than or equal to the log-likelihood for a given Φ and other parameters
- ELBO (Evidence Lower Bound)

Nonlinear Latent Variable Model - ELBO

- ELBO (Evidence Lower Bound) - Derivation

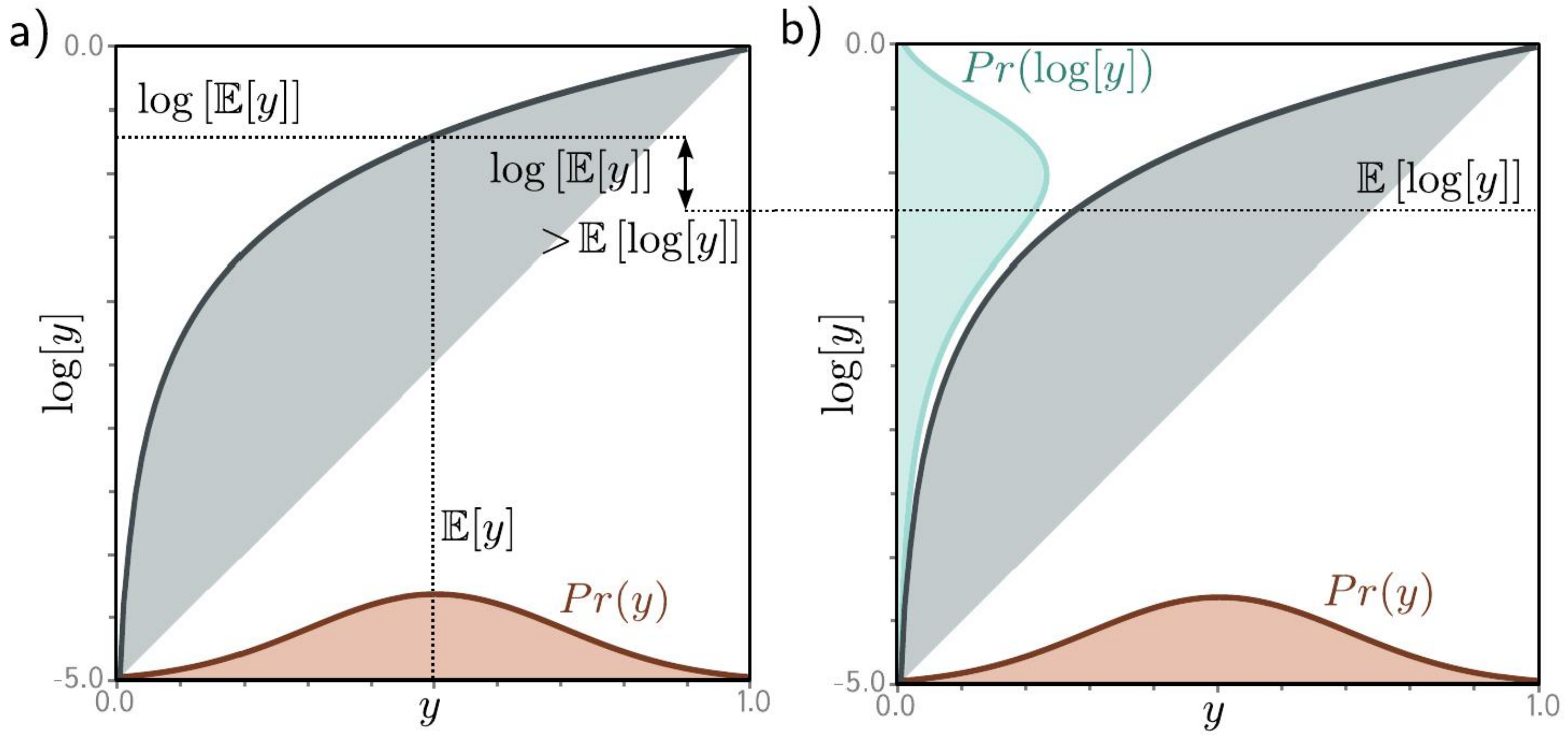
$$g[\mathbb{E}[y]] \geq \mathbb{E}\big[g[y]\big]$$

$$\log\big[\mathbb{E}[y]\big] \geq \mathbb{E}\big[\log[y]\big]$$

Jensen Inequality
(Concave Function)

$$\log\left[\int Pr(y)h[y]dy\right] \geq \int Pr(y)\log[h[y]]dy$$

Expansion



Nonlinear Latent Variable Model - ELBO

- ELBO (Evidence Lower Bound) - Derivation

$$\begin{aligned}\log[Pr(\mathbf{x}|\boldsymbol{\phi})] &= \log\left[\int Pr(\mathbf{x},\mathbf{z}|\boldsymbol{\phi})d\mathbf{z}\right] \\ &= \log\left[\int q(\mathbf{z})\frac{Pr(\mathbf{x},\mathbf{z}|\boldsymbol{\phi})}{q(\mathbf{z})}d\mathbf{z}\right]\end{aligned}$$

multiply & divide by arbitrary probability distribution over latent i.e., *q*(z)

$$\log\left[\int q(\mathbf{z})\frac{Pr(\mathbf{x},\mathbf{z}|\boldsymbol{\phi})}{q(\mathbf{z})}d\mathbf{z}\right] \geq \underbrace{\int q(\mathbf{z})\log\left[\frac{Pr(\mathbf{x},\mathbf{z}|\boldsymbol{\phi})}{q(\mathbf{z})}\right]d\mathbf{z}}_{\text{Evidence lower bound}}$$

using Jensen's inequality

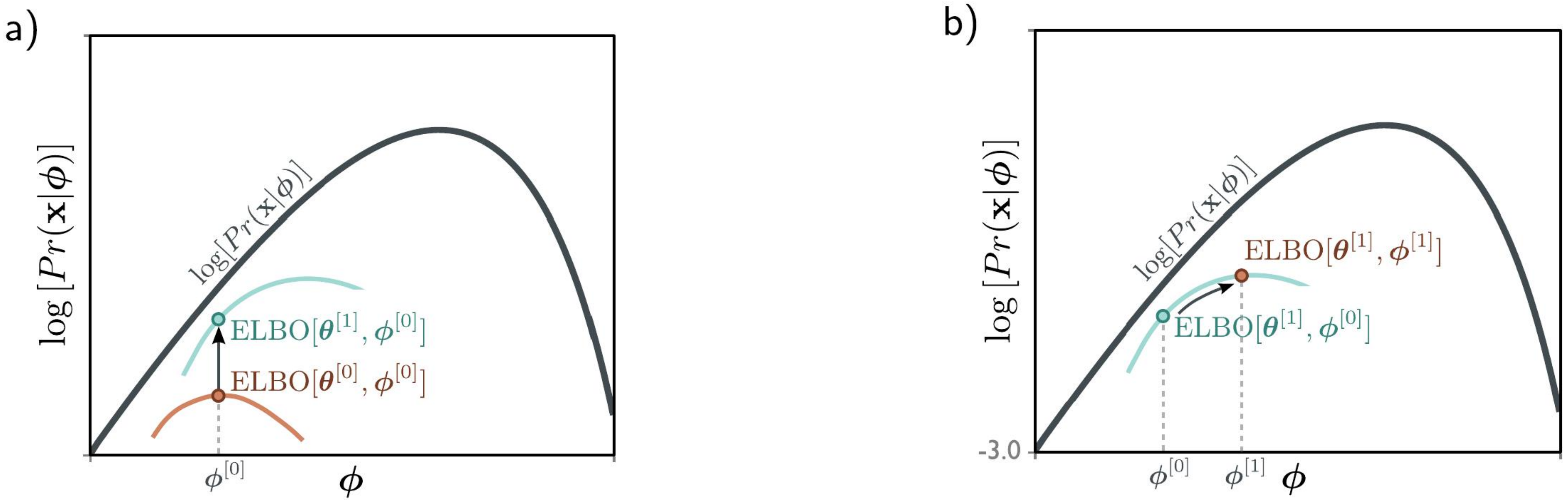
- In practice $q(\mathbf{z})$ is parameterized by $\boldsymbol{\theta}$

$$\text{ELBO}[\boldsymbol{\theta},\boldsymbol{\phi}] = \int q(\mathbf{z}|\boldsymbol{\theta})\log\left[\frac{Pr(\mathbf{x},\mathbf{z}|\boldsymbol{\phi})}{q(\mathbf{z}|\boldsymbol{\theta})}\right]d\mathbf{z}$$

maximize w.r.t both $\boldsymbol{\theta}$ and $\boldsymbol{\phi}$

Nonlinear Latent Variable Model - **ELBO**

$$\hat{\phi} = \underset{\phi}{\operatorname{argmax}} \left[\sum_{i=1}^{I} \log\left[Pr(\mathbf{x}_i|\phi) \right] \right]$$



- **Objective** : maximize the log-likelihood (black curve) with respect to the parameters ϕ
- For fixed θ, we get a function of ϕ (two colored curves for different values of θ)
- The log-likelihood can be increased by either ways

Nonlinear Latent Variable Model - ELBO

- **Tight ELBO** - ELBO concide with the likelihood function
  - for a fixed $\boldsymbol{\Phi}$

$$\begin{aligned}
\text{ELBO}[\boldsymbol{\theta}, \phi] &= \int q(\mathbf{z}|\boldsymbol{\theta}) \log\left[\frac{Pr(\mathbf{x}, \mathbf{z}|\phi)}{q(\mathbf{z}|\boldsymbol{\theta})}\right] d\mathbf{z} \\
&= \int q(\mathbf{z}|\boldsymbol{\theta}) \log\left[\frac{Pr(\mathbf{z}|\mathbf{x}, \phi)Pr(\mathbf{x}|\phi)}{q(\mathbf{z}|\boldsymbol{\theta})}\right] d\mathbf{z} \\
&= \int q(\mathbf{z}|\boldsymbol{\theta}) \log\big[Pr(\mathbf{x}|\phi)\big] d\mathbf{z} + \int q(\mathbf{z}|\boldsymbol{\theta}) \log\left[\frac{Pr(\mathbf{z}|\mathbf{x}, \phi)}{q(\mathbf{z}|\boldsymbol{\theta})}\right] d\mathbf{z} \\
&= \log\big[Pr(\mathbf{x}|\phi)\big] + \int q(\mathbf{z}|\boldsymbol{\theta}) \log\left[\frac{Pr(\mathbf{z}|\mathbf{x}, \phi)}{q(\mathbf{z}|\boldsymbol{\theta})}\right] d\mathbf{z} \\
&= \log\big[Pr(\mathbf{x}|\phi)\big] - \mathrm{D}_{KL}\Big[q(\mathbf{z}|\boldsymbol{\theta}) \Big|\Big| \boxed{Pr(\mathbf{z}|\mathbf{x}, \phi)}\Big].
\end{aligned}$$

conditional probability

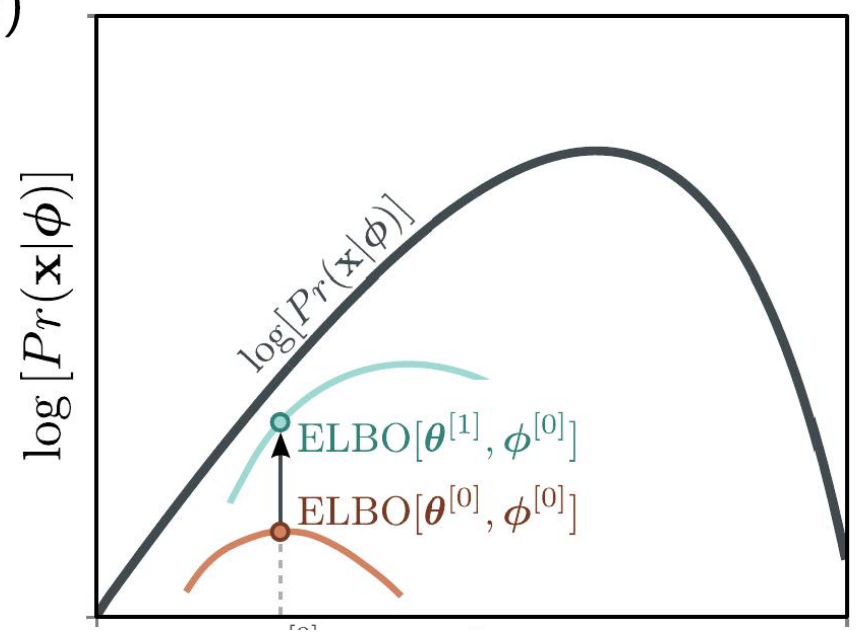
posterior distribution

Kullback-Leibler (KL) Divergence (Measures the distance between two distributions)

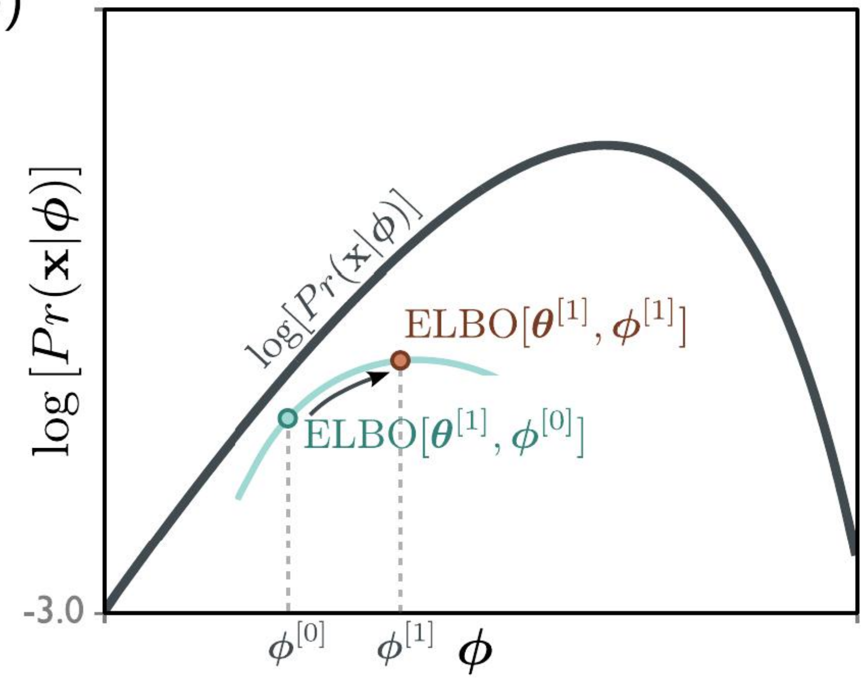
the bound is tight, when KL distance is zero i.e.,

$$q(\mathbf{z}|\boldsymbol{\theta}) = Pr(\mathbf{z}|\mathbf{x}, \phi)$$

a)



b)



Nonlinear Latent Variable Model - **ELBO**

- ELBO as reconstruction loss - KL distance to prior

$$
\begin{aligned}
\mathrm{ELBO}[\boldsymbol{\theta}, \boldsymbol{\phi}] &= \int q(\mathbf{z}|\boldsymbol{\theta}) \log\left[\frac{Pr(\mathbf{x},\mathbf{z}|\boldsymbol{\phi})}{q(\mathbf{z}|\boldsymbol{\theta})}\right] d\mathbf{z} \\
&= \int q(\mathbf{z}|\boldsymbol{\theta}) \log\left[\frac{Pr(\mathbf{x}|\mathbf{z},\boldsymbol{\phi})Pr(\mathbf{z})}{q(\mathbf{z}|\boldsymbol{\theta})}\right] d\mathbf{z} \\
&= \int q(\mathbf{z}|\boldsymbol{\theta}) \log\left[Pr(\mathbf{x}|\mathbf{z},\boldsymbol{\phi})\right] d\mathbf{z} + \int q(\mathbf{z}|\boldsymbol{\theta}) \log\left[\frac{Pr(\mathbf{z})}{q(\mathbf{z}|\boldsymbol{\theta})}\right] d\mathbf{z} \\
&= \int q(\mathbf{z}|\boldsymbol{\theta}) \log\left[\boxed{Pr(\mathbf{x}|\mathbf{z},\boldsymbol{\phi})}\right] d\mathbf{z} - \underbrace{\mathrm{D}_{KL}\left[q(\mathbf{z}|\boldsymbol{\theta}) \middle|\middle| Pr(\mathbf{z})\right],}
\end{aligned}
$$

conditional probability

reconstruction accuracy

degree of agreement between auxiliary distribution and prior

This formulation is generally used in the **variational autoencoder**

Nonlinear Latent Variable Model - ELBO

- Tight ELBO - ELBO concide with the likelihood function
  - for a fixed ***Φ***

$$q(\mathbf{z}|\boldsymbol{\theta}) = Pr(\mathbf{z}|\mathbf{x}, \phi)$$

$$Pr(\mathbf{z}|\mathbf{x}, \phi) = \frac{Pr(\mathbf{x}|\mathbf{z}, \phi)Pr(\mathbf{z})}{\boxed{Pr(\mathbf{x}|\phi)}}$$

Baye’s rule

intractable, we can’t evaluate this

Solution ?

multivariate normal distribution mean *μ* and diagonal variance *Σ*

- **Solution** : make a variational approximation
- Choose a **simple auxiliary distribution** $\boxed{q(\mathbf{z} \mid \theta)}$ to approximate **true posterior**

during training the goal is to find values of *μ* and *Σ*
such that the normal distrubution is close to the true posterior *Pr(***z** | **x***)*

= minimize the KL divergence

$$q(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}) = \mathrm{Norm}_{\mathbf{z}}\left[\underbrace{\mathbf{g}_{\boldsymbol{\mu}}[\mathbf{x}, \boldsymbol{\theta}], \mathbf{g}_{\boldsymbol{\Sigma}}[\mathbf{x}, \boldsymbol{\theta}]}\right]$$

Neural network with params **θ**

The Variational Autoencoder

$$\mathrm{ELBO}[\boldsymbol{\theta}, \boldsymbol{\phi}] = \underbrace{\int q(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}) \log\left[Pr(\mathbf{x}|\mathbf{z}, \boldsymbol{\phi})\right] d\mathbf{z}}_{\text{Intractable Integral}} - \mathrm{D}_{KL}\left[q(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}) \middle|\middle| Pr(\mathbf{z})\right]$$

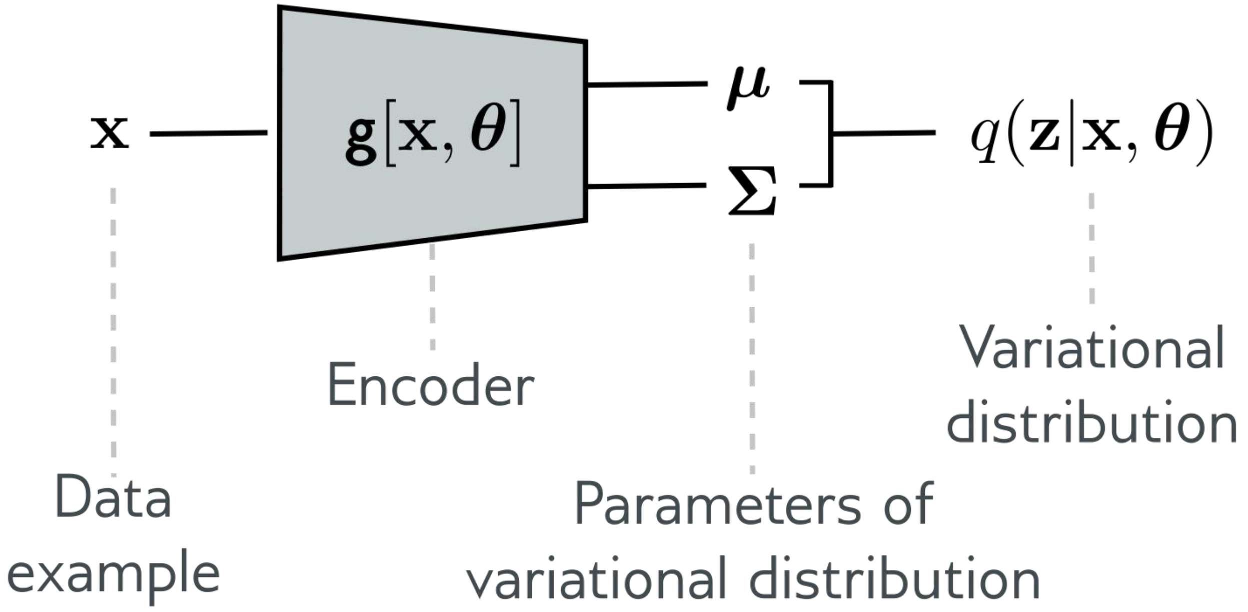
Solution : approximate it by sampling i.e., take a Monte Carlo estimate

$$\mathrm{ELBO}[\boldsymbol{\theta}, \boldsymbol{\phi}] \approx \log\left[Pr(\mathbf{x}|\mathbf{z}^*, \boldsymbol{\phi})\right] - \mathrm{D}_{KL}\left[q(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}) \middle|\middle| Pr(\mathbf{z})\right]$$

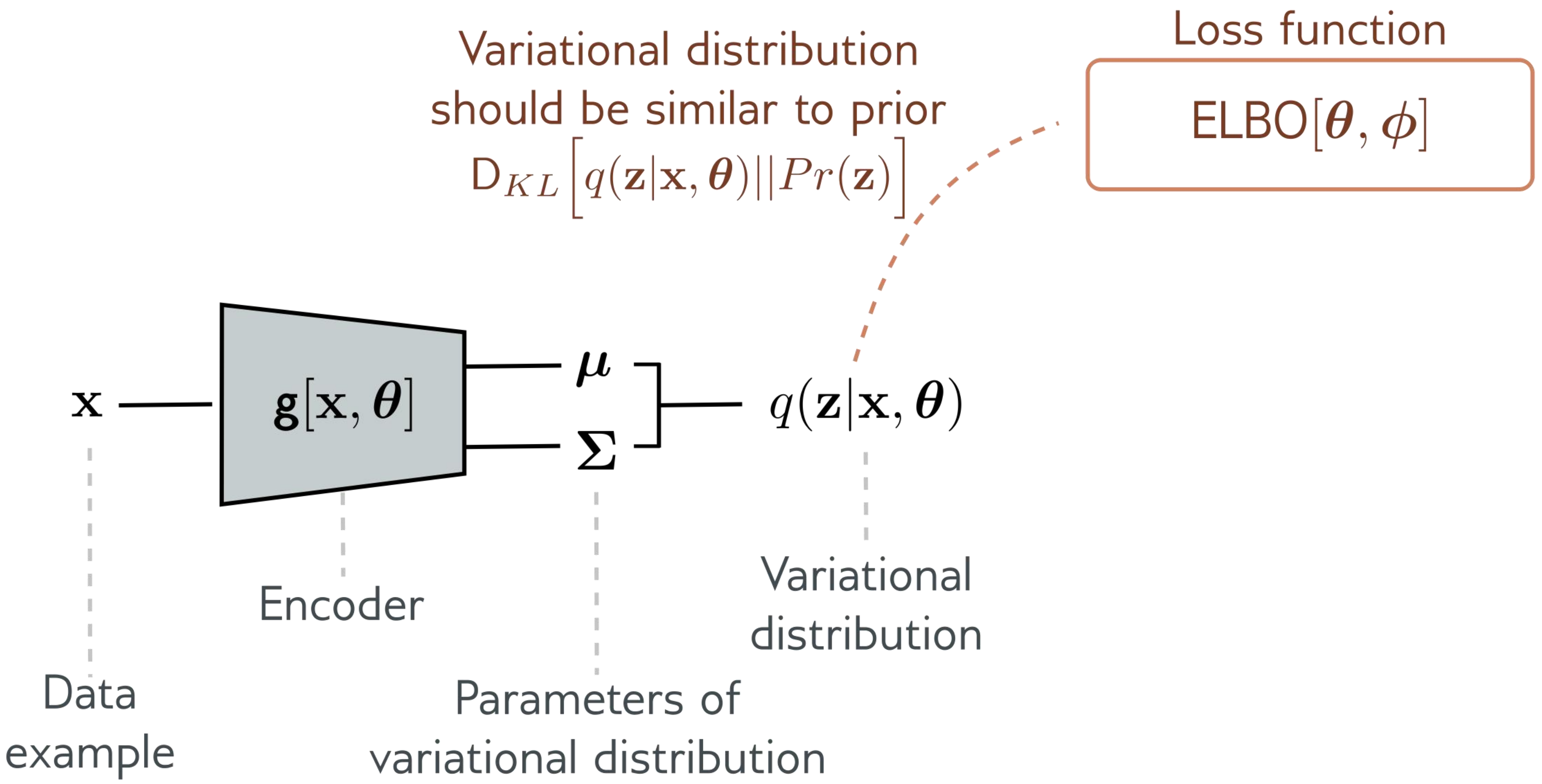
$$\mathrm{D}_{KL}\left[q(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}) \middle|\middle| Pr(\mathbf{z})\right] = \frac{1}{2}\left(\mathrm{Tr}[\boldsymbol{\Sigma}] + \boldsymbol{\mu}^T\boldsymbol{\mu} - \boxed{D_{\mathbf{z}}} - \log\left[\det[\boldsymbol{\Sigma}]\right]\right)$$

Dimensionality of the latent space

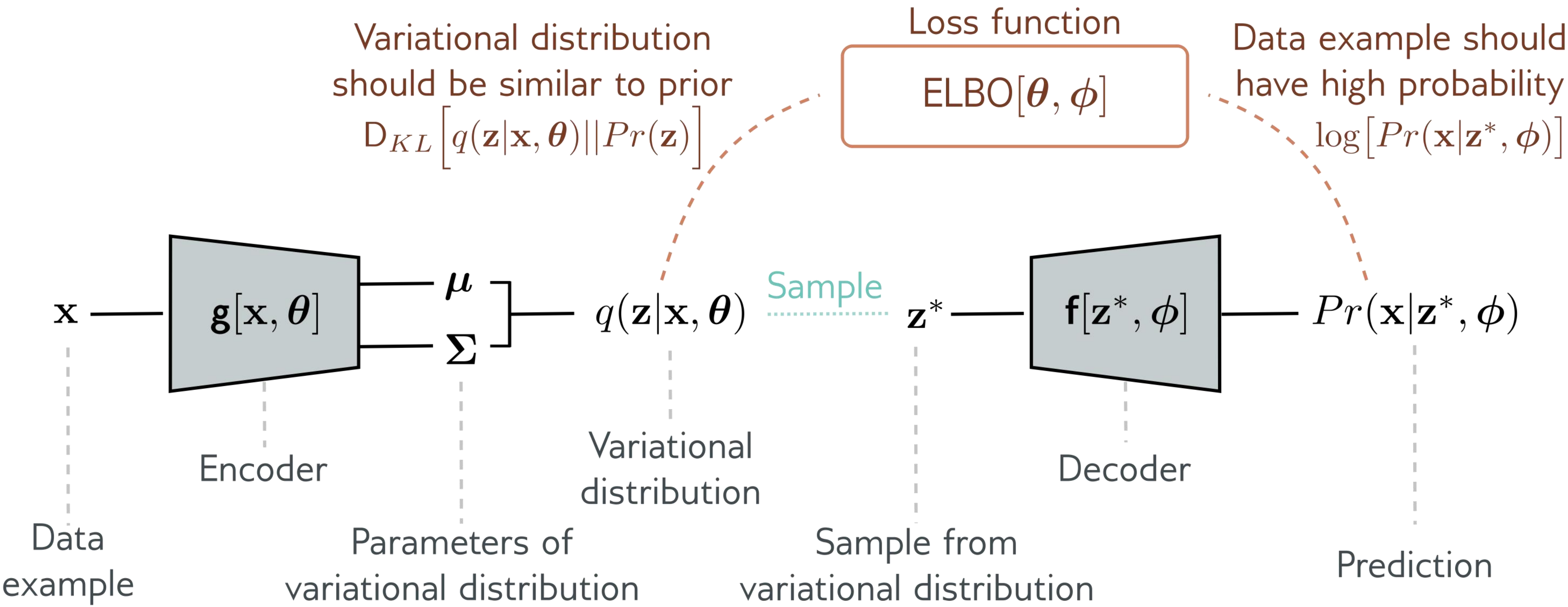
The Variational Autoencoder



The Variational Autoencoder



The Variational Autoencoder



Vector Quantised
Variational Autoencoder (VAE)

The VQVAE - Vector Quantized VAE

The Vector Quantised- Variational AutoEncoder (VQ-VAE), differs from VAEs in two key ways:

- the encoder network outputs discrete, rather than continuous codes
- the prior is learnt rather than static

Neural Discrete Representation Learning

Aaron van den Oord
DeepMind
avdnoord@google.com

Oriol Vinyals
DeepMind
vinyals@google.com

Koray Kavukcuoglu
DeepMind
korayk@google.com

Van Den Oord, Aaron, and Oriol Vinyals. "Neural discrete representation learning." Advances in neural information processing systems 30 (2017).

The VQVAE - Vector Quantized VAE

Key Idea :

- Incorporate ideas from vector quantisation (VQ)
- VQ method allows model to circumvent issues of “posterior collapse”
- where the latents are ignored when they are paired with a powerful autoregressive decoder =
- typically observed in the VAE framework.

VAE setup

- Posterior Distribution $q(z|x)$
- Prior Distribution $p(z)$
- Decoder with distribution $p(x|z)$

Posterior and prior are assumed normally distributed

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The VQVAE - Vector Quantized VAE

VQ-VAE:

- Discrete latent variables
- New way of training leveraging the concepts from vector quantisation (VQ)
- Posterior and prior distributions are categorical

Van Den Oord, Aaron, and Oriol Vinyals. "Neural discrete representation learning." Advances in neural information processing systems 30 (2017).

The VQVAE - Formulation

Discrete Latent Variables

Define a latent embedding space $e \in R^{K \times D}$
K : Size of the discrete latent space (K-way categorical)

D is the dimensionality of each latent embedding vector

$$e_i \in R^D, i \in 1, 2, ..., K$$

The encoder takes an input and produce output $z_e(x)$

Discrete latent variable is then calculated by a nearest neighbour look-up using a shared embedding space

$$q(z = k|x) = \begin{cases} 1 & \text{for } \mathrm{k} = \mathrm{argmin}_j \|z_e(x) - e_j\|_2 \\ 0 & \text{otherwise} \end{cases}$$

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The VQVAE - Formulation

the posterior is a categorical distribution as one-hot

$$q(z = k|x) = \begin{cases} 1 & \text{for } \ \mathrm{k} = \mathrm{argmin}_j \|z_e(x) - e_j\|_2 \\ 0 & \text{otherwise} \end{cases}$$

Decoder input is the embedding vector calculated from NN search

$$z_q(x) = e_k, \quad \text{where} \quad k = \mathrm{argmin}_j \|z_e(x) - e_j\|_2$$

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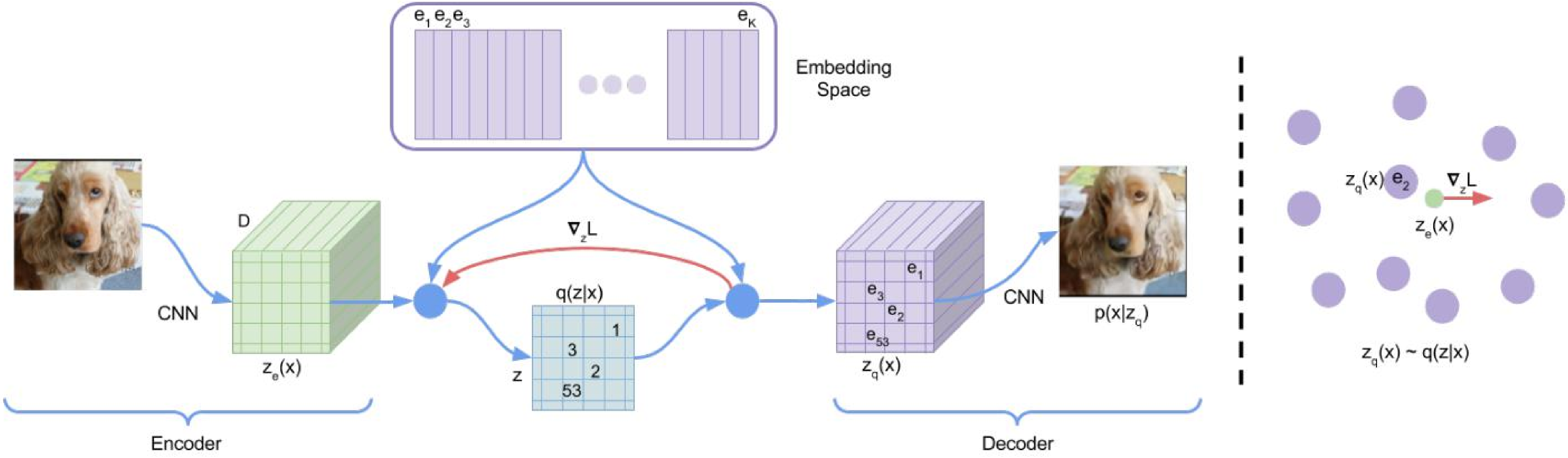
The VQVAE - Training



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The VQVAE - Training

There is no real gradient defined for the below equation,

$$z_q(x) = e_k, \quad \text{where} \quad k = \text{argmin}_j \|z_e(x) - e_j\|_2$$

however we approximate the gradient similar to the straight-through estimator

- copy gradients from decoder input to encoder output .

$$z_q(x) \qquad\qquad z_e(x)$$

- During forward computation the nearest embedding is passed to the decoder,

- During the backwards pass the gradient is passed unaltered to the encoder

Will this work ? Why?

- the output representation of the encoder and the input to the decoder share the same D dimensional space,

- the gradients contain useful information for how the encoder has to change its output to lower the reconstruction loss.

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The VQVAE - Training

- the gradient must push the encoder's output to be discretised differently in the next forward pass, because the assignment will be different

- Total Loss

$$L = \log p(x|z_q(x)) + \|\text{sg}[z_e(x)] - e\|_2^2 + \beta\|z_e(x) - \text{sg}[e]\|_2^2$$

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The VQVAE - Training

- the gradient must push the encoder's output to be discretised differently in the next forward pass, because the assignment will be different

- Total Loss

reconstruction loss
Due to the straight-through gradient estimation of mapping from $z_e(x)$ to $z_q(x)$, the embeddings e_i receive no gradients from the reconstruction loss

$$L = \boxed{\log p(x|z_q(x))} + \boxed{\|\text{sg}[z_e(x)] - e\|_2^2} + \boxed{\beta \|z_e(x) - \text{sg}[e]\|_2^2}$$

VQ objective uses the l_2 error to move the embedding vectors e_i towards the encoder outputs $z_e(x)$

Commitment Loss
Volumne of the embedding space can grow arbitrarily. To make sure the encoder commits to an embedding and its output does not grow.

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The VQVAE - Results

Left: ImageNet 128x128x3 images, right: reconstructions from a VQ-VAE with a 32x32x1 latent space, with K=512.

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