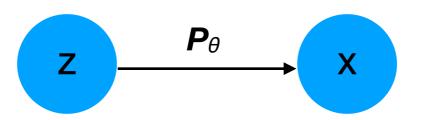
# CS/DS 552: Class 4

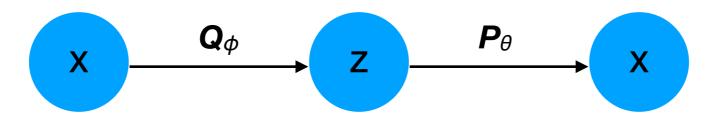
Jacob Whitehill

# Variational autoencoders (VAEs)

- Fundamentally, a VAE is an LVM, where we posit that each
   x is "generated" by a latent code z:
  - 1. Sample  $\mathbf{z} \sim P(\mathbf{z}) \in \mathbb{R}^d$  using an easy-to-sample  $P(\mathbf{z})$ .
  - 2. Compute  $\mathbf{x} = P_{\theta}(\mathbf{x} \mid \mathbf{z}) \in \mathbb{R}^m$ , where g is some "decoder" function with parameters  $\theta$ .

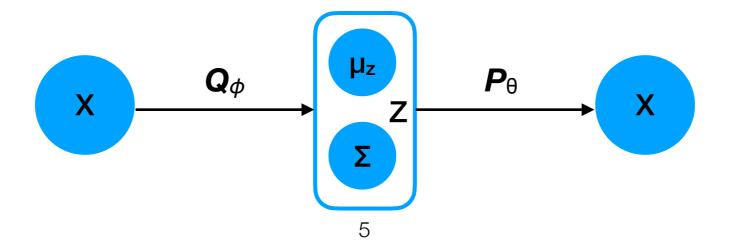


- Architecturally, however, and because of how it is trained, a VAE consists of an encoder NN  $Q_{\phi}$  and decoder NN  $P_{\theta}$ .
  - $Q_{\phi}(\mathbf{z} \mid \mathbf{x})$  outputs a probability distribution over **Z** given **X**.
  - $P_{\theta}(\mathbf{x} \mid \mathbf{z})$  outputs a probability distribution over **X** given **Z**.



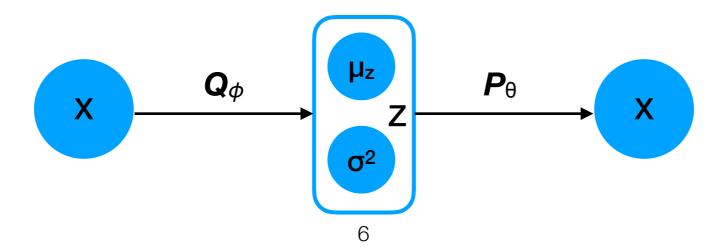
#### VAE architecture: encoder

- Most commonly,  $Q_{\phi}$  is constrained to output a Gaussian distribution over latent codes **z** given input **x**.
- How do we force  $Q_{\phi}$  to output a Gaussian distribution?
  - Given  $\mathbf{x}$ ,  $Q_{\phi}$  needs to output:
    - Mean µz
    - Covariance matrix Σ



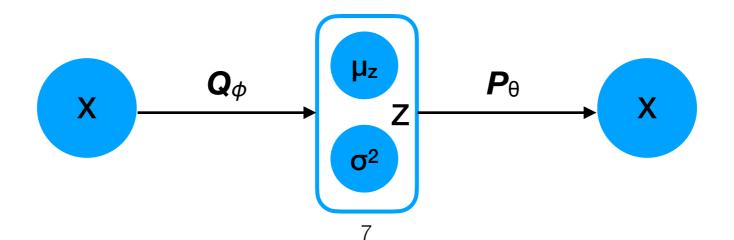
### VAE architecture: encoder

• As a simplification,  $Q_{\phi}$  can output a diagonal covariance matrix parameterized by just a vector [  $\sigma_1^2$ , ...,  $\sigma_d^2$  ].



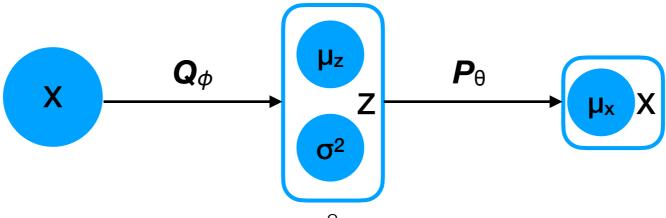
### VAE architecture: encoder

- As a simplification,  $Q_{\phi}$  can output a diagonal covariance matrix parameterized by just a vector [  $\sigma_1^2$ , ...,  $\sigma_d^2$  ].
- All in all,  $Q_{\phi}$  outputs 2d entries, where the first d specify the mean and the second d specify the covariance.
- We must force positivity of  $[\sigma_{1}^{2}, ..., \sigma_{d}^{2}]$ , e.g., by exponentiating the output of  $Q_{\phi}$ .

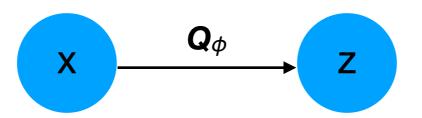


### VAE architecture: decoder

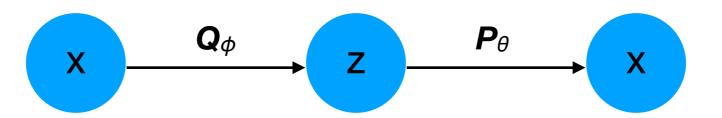
- $P_{\theta}$  is usually one of:
  - 1. Gaussian  $\mathcal{N}(\mu_{\mathbf{x}},\mathbf{I})$  with mean  $\mu_{\mathbf{x}}$  and I-covariance
    - Useful for predicting data from  $\mathbb{R}^m$ .
    - NN: no activation function.
  - 2. Element-wise Bernoulli with mean  $\mu_x$ .
    - Useful for predicting data from  $[0,1]^m$ .
    - NN: logistic activation function.



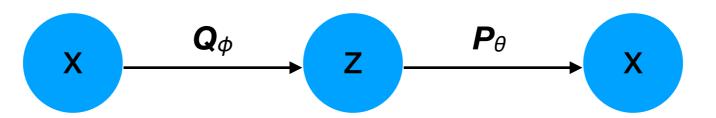
• With  $Q_{\phi}$ , we can estimate from input  $\mathbf{x} \in \mathbb{R}^m$  the latent code  $\mathbf{z} \in \mathbb{R}^d$  that generated it.



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- With  $P_{\theta}$ , we can use input code  $\mathbf{z} \in \mathbb{R}^d$  to generate  $\mathbf{x} \in \mathbb{R}^m$ .

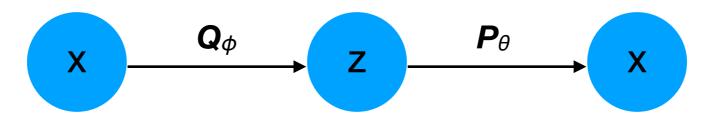


- With  $Q_{\phi}$ , we can estimate from input  $\mathbf{x} \in \mathbb{R}^m$  the latent code  $\mathbf{z} \in \mathbb{R}^d$  that generated it.
- With  $P_{\theta}$ , we can use input code  $\mathbf{z} \in \mathbb{R}^d$  to generate  $\mathbf{x} \in \mathbb{R}^m$ .
- $P(\mathbf{x} \mid \mathbf{z})$  represents how likely the VAE believes a particular example  $\mathbf{x}$  is to be generated from latent code  $\mathbf{z}$ .
- For good reconstruction quality, we want  $P(\mathbf{x} \mid \mathbf{z}) = P_{\theta}(Q_{\phi}(\mathbf{x}))$  to be *high*.



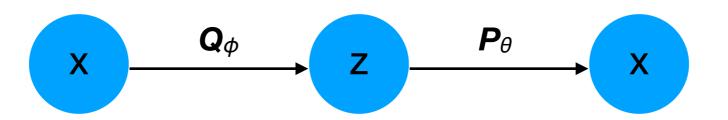
# NN implementations

- VAEs can be applied to many types of data (images, tabular data, time series, ...) given an appropriate architecture, e.g.:
  - FCNN encoder & decoder for tabular data.
  - Conv. encoder & de-conv. decoder for images.
  - RNN encoder & decoder for time series.



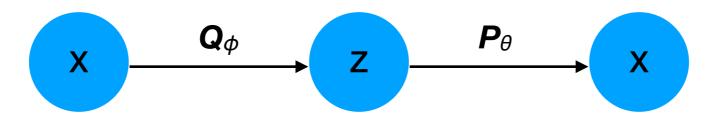
# Likelihood models & loss functions

- The VAE decoder is usually one of:
  - Gaussian  $P(\mathbf{x} \mid \mathbf{z}) = \mathcal{N}(\mu_{\mathbf{x}}, \mathbf{I})$ , where  $\mu_{\mathbf{x}} \in \mathbb{R}^m$ .
  - Bernoulli  $P(\mathbf{x} \mid \mathbf{z}) = \text{Ber}(\mu_{\mathbf{x}})$ , where  $\mu_{\mathbf{x}} \in [0,1]^m$ .



# Likelihood models & loss functions

- This requires an activation at the end of the decoder:
  - Gaussian: identity/nothing
  - Bernoulli: logistic sigmoid



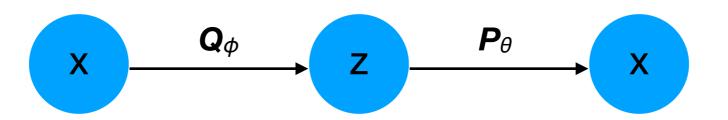
# Likelihood models & loss functions

Maximizing the likelihood = Minimizing a loss function:

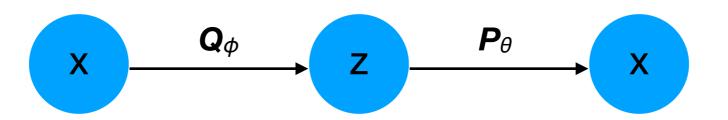
• Gaussian: MSE: 
$$\frac{1}{2}||x - \mu_{\mathbf{x}}||^2$$

• Bernoulli: BCE:  $-y \log \hat{y} - (1-y) \log(1-\hat{y})$ 

Binary cross-entropy



- The parameters  $\phi$  and  $\theta$  are trained using maximum-likelihood estimation (MLE).
- We aim to maximize the likelihood of our observed training data, given P's parameters  $\theta$ , i.e.:  $P_{\theta}(\{\mathbf{x}^{(i)}\}_{i=1}^n)$
- Using a MLE approximation technique, we will also optimize Q's parameters  $\phi$  along the way.



- Define networks  $Q_{\phi}$  and decoder  $P_{\theta}$ .
- Initialize parameters  $\phi$  and  $\theta$ .

$$\mathcal{N}(\epsilon;\mathbf{0},\mathbf{I})\leadsto\epsilon$$
  $\mathbf{x} \xrightarrow[Q_{\phi}(\mathbf{z}|\mathbf{x})]{} (\mu,\sigma^2) \xrightarrow{} \epsilon\odot\sigma + \mu \to P_{ heta}(\mathbf{x}\mid\mathbf{z})$  Input Hidden 17 Output

- Define networks  $Q_{\phi}$  and decoder  $P_{\theta}$ .
- Initialize parameters  $\phi$  and  $\theta$ .
- For each mini-batch:
  - Select  $\tilde{n}$  examples:  $\{\mathbf{x}^{(i)}\}_{i=1}^{\tilde{n}} \subset \mathbb{R}^m$

$$\mathcal{N}(\epsilon;\mathbf{0},\mathbf{I})\leadsto\epsilon$$
  $\mathbf{x} \xrightarrow[Q_{\phi}(\mathbf{z}|\mathbf{x})]{} (\mu,\sigma^2) \xrightarrow{} \epsilon\odot\sigma + \mu \rightarrow P_{\theta}(\mathbf{x}\mid\mathbf{z})$  Input Hidden 18 Output

- Define networks  $Q_{\phi}$  and decoder  $P_{\theta}$ .
- Initialize parameters  $\phi$  and  $\theta$ .
- For each mini-batch:
  - Select  $\tilde{n}$  examples:  $\{\mathbf{x}^{(i)}\}_{i=1}^{\tilde{n}} \subset \mathbb{R}^m$
  - Sample  $\tilde{n}$  noise vectors:  $\{\epsilon^{(i)}\}_{i=1}^{\tilde{n}} \subset \mathbb{R}^d$

$$\mathcal{N}(\epsilon;\mathbf{0},\mathbf{I})\leadsto\epsilon$$
  $\mathbf{x} \xrightarrow[Q_{\phi}(\mathbf{z}|\mathbf{x})]{} (\mu,\sigma^2) \xrightarrow{} \epsilon\odot\sigma + \mu \rightarrow P_{\theta}(\mathbf{x}\mid\mathbf{z})$  Input Hidden 19 Output

- Define networks  $Q_{\phi}$  and decoder  $P_{\theta}$ .
- Initialize parameters  $\phi$  and  $\theta$ .
- For each mini-batch:
  - Select  $\tilde{n}$  examples:  $\{\mathbf{x}^{(i)}\}_{i=1}^{\tilde{n}} \subset \mathbb{R}^m$
  - Sample  $\tilde{n}$  noise vectors:  $\{\epsilon^{(i)}\}_{i=1}^{\tilde{n}} \subset \mathbb{R}^d$
  - Compute:  $(\mu^{(i)}, \sigma^{(i)})^2 = Q_{\phi}(\mathbf{z}^{(i)} \mid \mathbf{x}^{(i)}), \ \forall i$

$$\mathcal{N}(\epsilon;\mathbf{0},\mathbf{I})\leadsto \epsilon$$
  $\mathbf{x} \xrightarrow[Q_{\phi}(\mathbf{z}|\mathbf{x})]{} (\mu,\sigma^2) \xrightarrow{} \epsilon\odot\sigma + \mu \to P_{ heta}(\mathbf{x}\mid\mathbf{z})$  Input Hidden 20 Output

Input Hidden

- Define networks  $Q_{\phi}$  and decoder  $P_{\theta}$ .
- Initialize parameters  $\phi$  and  $\theta$ .
- For each mini-batch:
  - Select  $\tilde{n}$  examples:  $\{\mathbf{x}^{(i)}\}_{i=1}^{\tilde{n}} \subset \mathbb{R}^m$
  - Sample  $\tilde{n}$  noise vectors:  $\{\epsilon^{(i)}\}_{i=1}^{\tilde{n}} \subset \mathbb{R}^d$
  - Compute:  $(\mu^{(i)}, \sigma^{(i)})^2 = Q_{\phi}(\mathbf{z}^{(i)} \mid \mathbf{x}^{(i)}), \ \forall i$
  - Compute:  $\mathbf{z}^{(i)} = \epsilon^{(i)} \odot \sigma^{(i)} + \mu^{(i)}$

$$\mathbf{x} \underset{Q_{\phi}(\mathbf{z}|\mathbf{x})}{\longrightarrow} (\mu, \sigma^2) \to \epsilon \odot \sigma + \mu \to P_{\theta}(\mathbf{x} \mid \mathbf{z})$$

Input Hidden 21 Output

- Define networks  $Q_{\phi}$  and decoder  $P_{\theta}$ .
- Initialize parameters  $\phi$  and  $\theta$ .
- For each mini-batch:
  - Select  $\tilde{n}$  examples:  $\{\mathbf{x}^{(i)}\}_{i=1}^{\tilde{n}} \subset \mathbb{R}^m$
  - Sample  $\tilde{n}$  noise vectors:  $\{\epsilon^{(i)}\}_{i=1}^{\tilde{n}} \subset \mathbb{R}^d$
  - Compute:  $(\mu^{(i)}, \sigma^{(i)}^2) = Q_{\phi}(\mathbf{z}^{(i)} \mid \mathbf{x}^{(i)}), \ \forall i$
  - Compute:  $\mathbf{z}^{(i)} = \epsilon^{(i)} \odot \sigma^{(i)} + \mu^{(i)}$
  - Maximize:

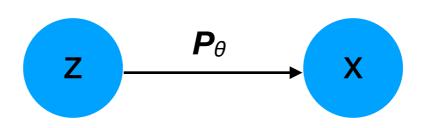
$$\log P_{\theta}(\mathbf{x}^{(i)} \mid \mathbf{z}^{(i)}) - D_{\mathrm{KL}}(Q_{\phi}(\mathbf{z}^{(i)}; \ \mathbf{x}^{(i)}) \parallel \mathcal{N}(\mathbf{z}; \mathbf{0}, \mathbf{I}))$$

- Define networks  $Q_{\phi}$  and decoder  $P_{\theta}$ .
- Initialize parameters  $\phi$  and  $\theta$ .
- For each mini-batch:
  - Select  $\tilde{n}$  examples:  $\{\mathbf{x}^{(i)}\}_{i=1}^{\tilde{n}} \subset \mathbb{R}^m$
  - Sample  $\tilde{n}$  noise vectors:  $\{\epsilon^{(i)}\}_{i=1}^{\tilde{n}} \subset \mathbb{R}^d$
  - Compute:  $(\mu^{(i)}, \sigma^{(i)}^2) = Q_{\phi}(\mathbf{z}^{(i)} \mid \mathbf{x}^{(i)}), \ \forall i$
  - Compute:  $\mathbf{z}^{(i)} = \epsilon^{(i)} \odot \sigma^{(i)} + \mu^{(i)}$
  - Maximize:

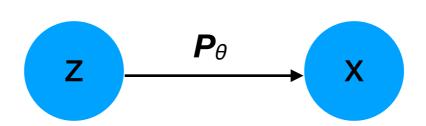
$$\log P_{\theta}(\mathbf{x}^{(i)} \mid \mathbf{z}^{(i)}) - D_{\mathrm{KL}}(Q_{\phi}(\mathbf{z}^{(i)}; \mathbf{x}^{(i)}) \parallel \mathcal{N}(\mathbf{z}; \mathbf{0}, \mathbf{I}))$$

• Update  $\phi$  and  $\theta$  using back-propagation.

$$\log P(\mathbf{x}) = \log \int_{\mathbf{z}} P(\mathbf{x}, \mathbf{z}) d\mathbf{z}$$

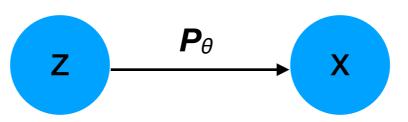


$$\begin{split} \log P(\mathbf{x}) &= \log \int_{\mathbf{z}} P(\mathbf{x}, \mathbf{z}) d\mathbf{z} \\ &= \log \int_{\mathbf{z}} P(\mathbf{x} \mid \mathbf{z}) P(\mathbf{z}) d\mathbf{z} \end{split} \quad \text{Definition of conditional probability} \end{split}$$



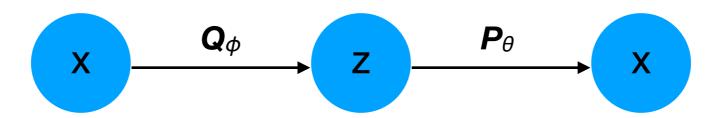
$$\log P(\mathbf{x}) = \log \int_{\mathbf{z}} P(\mathbf{x}, \mathbf{z}) d\mathbf{z}$$
$$= \log \int_{\mathbf{z}} P(\mathbf{x} \mid \mathbf{z}) P(\mathbf{z}) d\mathbf{z}$$

- We are in trouble!
  - This integral is the product of P(z) (e.g., Gaussian) and P(x | z) (i.e., the decoder NN). We cannot resolve it!
  - We cannot integrate numerically (intractable)!
- We cannot even evaluate  $P(\mathbf{x})$ , let alone optimize it!

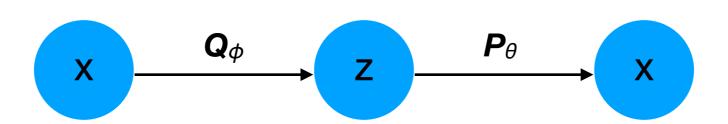


$$\log P(\mathbf{x}) = \log \int_{\mathbf{z}} P(\mathbf{x}, \mathbf{z}) d\mathbf{z}$$
$$= \log \int_{\mathbf{z}} P(\mathbf{x} \mid \mathbf{z}) P(\mathbf{z}) d\mathbf{z}$$

• By introducing auxiliary parameters  $\phi$  through an encoder network Q, we actually make the optimization easier...

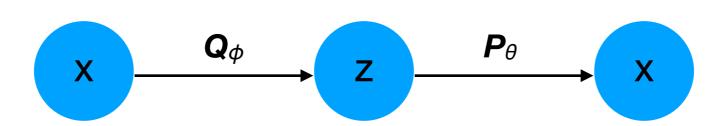


$$\begin{split} \log P(\mathbf{x}) &= \log \int_{\mathbf{z}} P(\mathbf{x}, \mathbf{z}) d\mathbf{z} \\ &= \log \int_{\mathbf{z}} P(\mathbf{x} \mid \mathbf{z}) P(\mathbf{z}) d\mathbf{z} \\ &= \log \int_{\mathbf{z}} Q(\mathbf{z} \mid \mathbf{x}) \frac{P(\mathbf{x} \mid \mathbf{z}) P(\mathbf{z})}{Q(\mathbf{z} \mid \mathbf{x})} d\mathbf{z} \end{split}$$
 This holds for any non-zero Q.



$$\begin{split} \log P(\mathbf{x}) &= \log \int_{\mathbf{z}} P(\mathbf{x}, \mathbf{z}) d\mathbf{z} \\ &= \log \int_{\mathbf{z}} P(\mathbf{x} \mid \mathbf{z}) P(\mathbf{z}) d\mathbf{z} \\ &= \log \int_{\mathbf{z}} Q(\mathbf{z} \mid \mathbf{x}) \frac{P(\mathbf{x} \mid \mathbf{z}) P(\mathbf{z})}{Q(\mathbf{z} \mid \mathbf{x})} d\mathbf{z} \quad \text{Note also that we can interpret this function as the expectation w.r.t. Q(z | x).} \end{split}$$

Note also that we can expectation w.r.t. Q(z | x).



$$\begin{split} \log P(\mathbf{x}) &= \log \int_{\mathbf{z}} P(\mathbf{x}, \mathbf{z}) d\mathbf{z} \\ &= \log \int_{\mathbf{z}} P(\mathbf{x} \mid \mathbf{z}) P(\mathbf{z}) d\mathbf{z} \\ &= \log \int_{\mathbf{z}} Q(\mathbf{z} \mid \mathbf{x}) \frac{P(\mathbf{x} \mid \mathbf{z}) P(\mathbf{z})}{Q(\mathbf{z} \mid \mathbf{x})} d\mathbf{z} \\ &\geq \int_{\mathbf{z}} Q(\mathbf{z} \mid \mathbf{x}) \log \left( P(\mathbf{x} \mid \mathbf{z}) \frac{P(\mathbf{z})}{Q(\mathbf{z} \mid \mathbf{x})} \right) d\mathbf{z} \quad \text{Jensen's inequality} \end{split}$$

This is called the Evidence Lower Bound (ELBO).

$$\begin{split} \log P(\mathbf{x}) &= \log \int_{\mathbf{z}} P(\mathbf{x}, \mathbf{z}) d\mathbf{z} \\ &= \log \int_{\mathbf{z}} P(\mathbf{x} \mid \mathbf{z}) P(\mathbf{z}) d\mathbf{z} \\ &= \log \int_{\mathbf{z}} Q(\mathbf{z} \mid \mathbf{x}) \frac{P(\mathbf{x} \mid \mathbf{z}) P(\mathbf{z})}{Q(\mathbf{z} \mid \mathbf{x})} d\mathbf{z} \\ &\geq \int_{\mathbf{z}} Q(\mathbf{z} \mid \mathbf{x}) \log \left( P(\mathbf{x} \mid \mathbf{z}) \frac{P(\mathbf{z})}{Q(\mathbf{z} \mid \mathbf{x})} \right) d\mathbf{z} \quad \text{Jensen's inequality} \end{split}$$

- It turns out (see Prince, sec. 17.4.1) that, if Q(z | x) = P(z), then this inequality is actually an equality.
- Hence, this lower-bound can actually be made "tight" if Q is powerful enough to approximate P(z).

$$\log P(\mathbf{x}) = \log \int_{\mathbf{z}} P(\mathbf{x}, \mathbf{z}) d\mathbf{z}$$

$$= \log \int_{\mathbf{z}} P(\mathbf{x} \mid \mathbf{z}) P(\mathbf{z}) d\mathbf{z}$$

$$= \log \int_{\mathbf{z}} Q(\mathbf{z} \mid \mathbf{x}) \frac{P(\mathbf{x} \mid \mathbf{z}) P(\mathbf{z})}{Q(\mathbf{z} \mid \mathbf{x})} d\mathbf{z}$$

$$\geq \int_{\mathbf{z}} Q(\mathbf{z} \mid \mathbf{x}) \log \left( P(\mathbf{x} \mid \mathbf{z}) \frac{P(\mathbf{z})}{Q(\mathbf{z} \mid \mathbf{x})} \right) d\mathbf{z}$$

$$= \int_{\mathbf{z}} Q(\mathbf{z} \mid \mathbf{x}) \log \frac{P(\mathbf{z})}{Q(\mathbf{z} \mid \mathbf{x})} d\mathbf{z} + \int_{\mathbf{z}} Q(\mathbf{z} \mid \mathbf{x}) \log P(\mathbf{x} \mid \mathbf{z}) d\mathbf{z}$$

$$\log P(\mathbf{x}) = \log \int_{\mathbf{z}} P(\mathbf{x}, \mathbf{z}) d\mathbf{z}$$

$$= \log \int_{\mathbf{z}} P(\mathbf{x} \mid \mathbf{z}) P(\mathbf{z}) d\mathbf{z}$$

$$= \log \int_{\mathbf{z}} Q(\mathbf{z} \mid \mathbf{x}) \frac{P(\mathbf{x} \mid \mathbf{z}) P(\mathbf{z})}{Q(\mathbf{z} \mid \mathbf{x})} d\mathbf{z}$$

$$\geq \int_{\mathbf{z}} Q(\mathbf{z} \mid \mathbf{x}) \log \left( P(\mathbf{x} \mid \mathbf{z}) \frac{P(\mathbf{z})}{Q(\mathbf{z} \mid \mathbf{x})} \right) d\mathbf{z}$$

$$= \int_{\mathbf{z}} Q(\mathbf{z} \mid \mathbf{x}) \log \frac{P(\mathbf{z})}{Q(\mathbf{z} \mid \mathbf{x})} d\mathbf{z} + \int_{\mathbf{z}} Q(\mathbf{z} \mid \mathbf{x}) \log P(\mathbf{x} \mid \mathbf{z}) d\mathbf{z}$$

$$= -D_{KL}(Q(\mathbf{z} \mid \mathbf{x}) \parallel P(\mathbf{z})) + \mathbb{E}_{Q}[\log P(\mathbf{x} \mid \mathbf{z})]$$

Definitions of KL-divergence and expectation.

## **ELBO**

- To maximize the ELBO, we need to:
  - Minimize KL-divergence of hidden state w.r.t. standard normal distribution.

and

Maximize the expected reconstruction log-likelihood.

$$\mathbf{x} \xrightarrow{\mathbf{Q}_{\phi}} \mathbf{z} \xrightarrow{\mathbf{P}_{\theta}} \mathbf{x}$$

$$= -D_{\mathrm{KL}}(Q_{\phi}(\mathbf{z} \mid \mathbf{x}) \parallel P(\mathbf{z})) + \mathbb{E}_{Q_{\phi}}[\log P_{\theta}(\mathbf{x} \mid \mathbf{z})]$$

## **ELBO**

The first term in the ELBO:

$$= -D_{\mathrm{KL}}(Q_{\phi}(\mathbf{z} \mid \mathbf{x}) \parallel P(\mathbf{z})) + \mathbb{E}_{Q_{\phi}}[\log P_{\theta}(\mathbf{x} \mid \mathbf{z})]$$

has closed-form differentiable solutions when  $P(\mathbf{z})$  and  $Q_{\phi}(\mathbf{z} \mid \mathbf{x})$  are Gaussian (see earlier slide).

#### **ELBO**

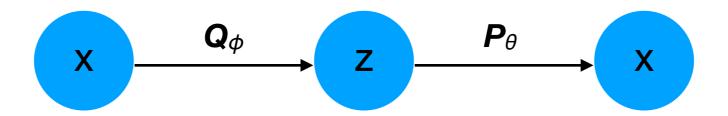
The second term in the ELBO:

$$= -D_{\mathrm{KL}}(Q_{\phi}(\mathbf{z} \mid \mathbf{x}) \parallel P(\mathbf{z})) + \mathbb{E}_{Q_{\phi}}[\log P_{\theta}(\mathbf{x} \mid \mathbf{z})]$$

can be approximated by sampling:

$$\mathbb{E}_{Q_{\phi}}[\log P_{\theta}(\mathbf{x} \mid \mathbf{z})] \approx \frac{1}{K} \sum_{k=1}^{K} \log P_{\theta}(\mathbf{x} \mid \mathbf{z}^{(k)})$$

where 
$$\mathbf{z}^{(k)} \sim Q_{\phi}(\mathbf{z} \mid \mathbf{x})$$

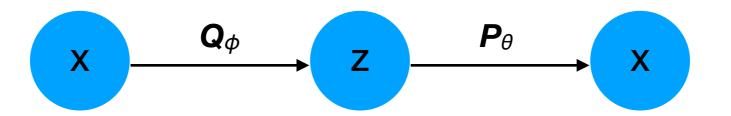


#### **ELBO**

- In particular:
  - 1. For input  $\mathbf{x}$ , compute  $Q(\mathbf{z} \mid \mathbf{x})$ .
  - 2. Sample K different  $\mathbf{z}^{(k)}$  from this distribution.
  - 3. For each  $\mathbf{z}^{(k)}$ , compute  $P(\mathbf{x} \mid \mathbf{z}^{(k)})$ , i.e., reconstruction probability of  $\mathbf{x}$  using  $\mathbf{z}$ .

$$\mathbb{E}_{Q_{\phi}}[\log P_{\theta}(\mathbf{x} \mid \mathbf{z})] \approx \frac{1}{K} \sum_{k=1}^{K} \log P_{\theta}(\mathbf{x} \mid \mathbf{z}^{(k)})$$

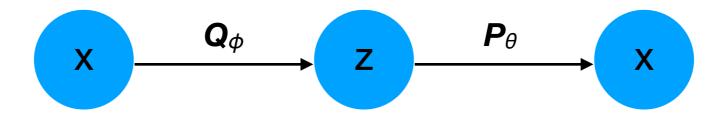
where 
$$\mathbf{z}^{(k)} \sim Q_{\phi}(\mathbf{z} \mid \mathbf{x})$$



### **ELBO**

• In practice, we usually set K=1 for simplicity.

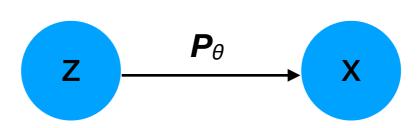
$$\mathbb{E}_{Q_{\phi}}[\log P_{\theta}(\mathbf{x} \mid \mathbf{z})] \approx \log P_{\theta}(\mathbf{x} \mid \mathbf{z})$$
where  $\mathbf{z} \sim Q_{\phi}(\mathbf{z} \mid \mathbf{x})$ 



Conceptually, we have changed from an optimization:

$$\underset{\theta}{\operatorname{arg}} \max_{f(\theta)} f(\theta)$$
 We cannot even evaluate  $f(\theta)$ 

to:



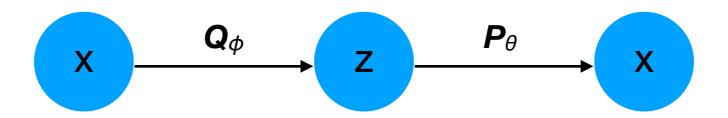
Conceptually, we have changed from an optimization:

$$\underset{\theta}{\operatorname{arg}} \max f(\theta)$$
 We cannot even evaluate  $f!$ 

to:

$$\underset{\theta,\phi}{\operatorname{arg}} \max_{g} g(\theta,\phi)$$
 We can both estimate and (using SGD) optimize  $g!$ 

where we can just discard  $\phi$  afterwards.



Conceptually, we have changed from an optimization:

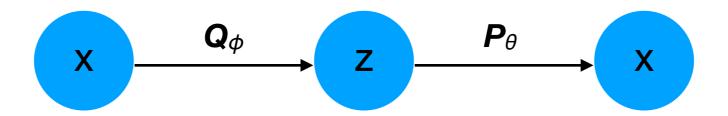
$$\underset{\theta}{\operatorname{arg}} \max f(\theta)$$
 We cannot even evaluate  $f!$ 

to:

$$\underset{\theta,\phi}{\operatorname{arg}} \max_{g} g(\theta,\phi)$$
 We can both estimate and (using SGD) optimize  $g!$ 

where we can just discard  $\phi$  afterwards.

Under what conditions can this actually work?



Conceptually, we have changed from an optimization:

$$\underset{\theta}{\operatorname{arg}} \max f(\theta)$$
 We cannot even evaluate  $f!$ 

to:

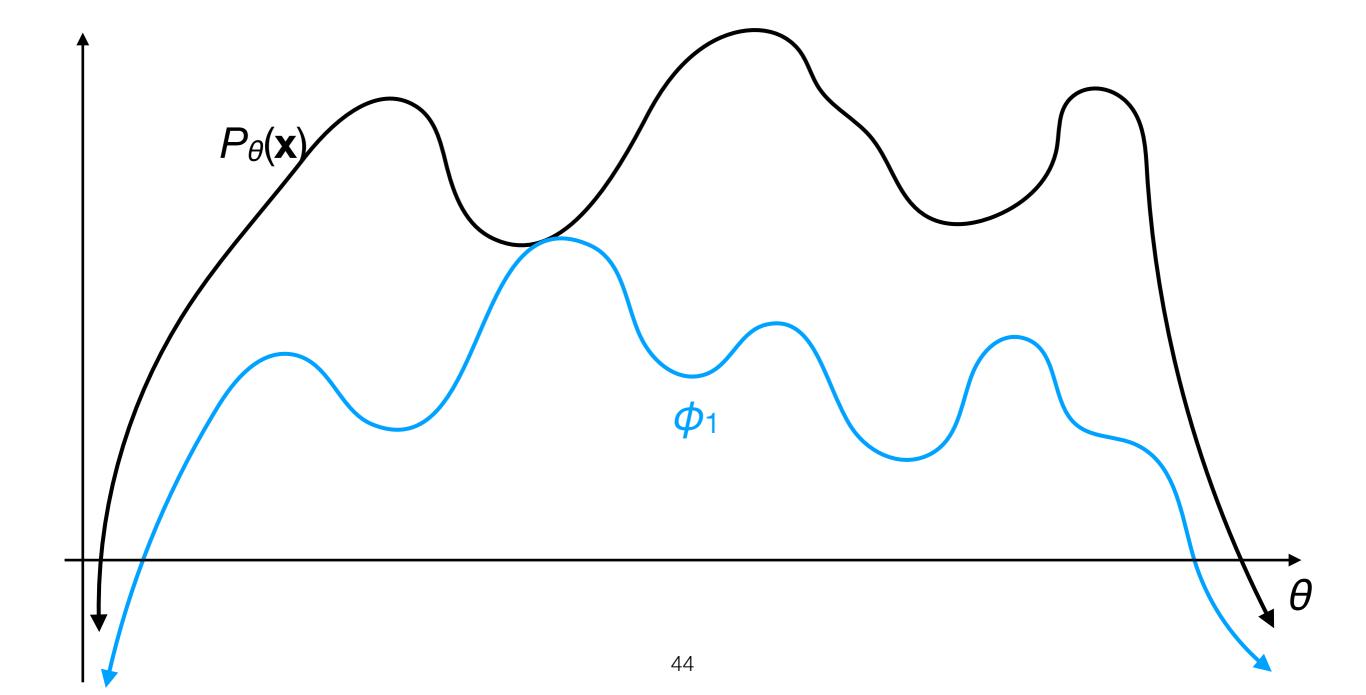
$$\underset{\theta,\phi}{\operatorname{arg}} \max_{g} g(\theta,\phi)$$
 We can both estimate and (using SGD) optimize  $g!$ 

where we can just discard  $\phi$  afterwards.

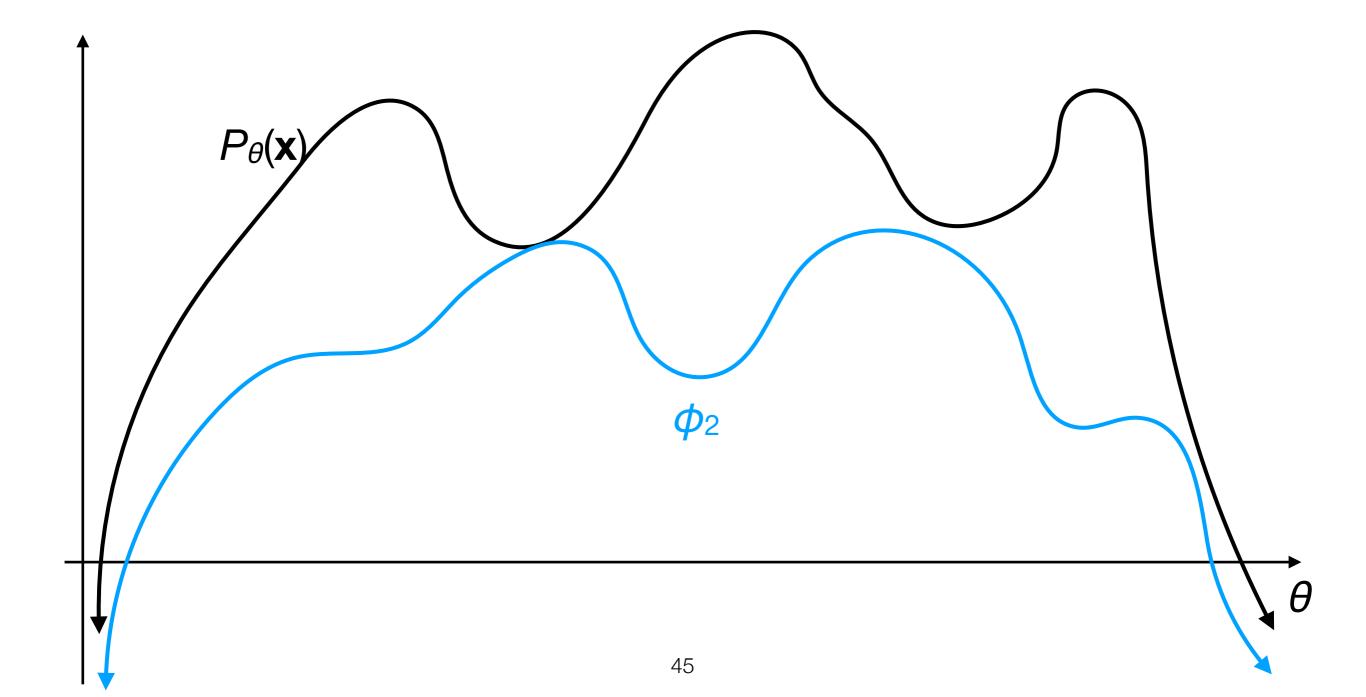
- Under what conditions can this actually work?
  - 1. *g* is a lower bound for *f*.
  - 2. This lower bound can be made "tight" to f.



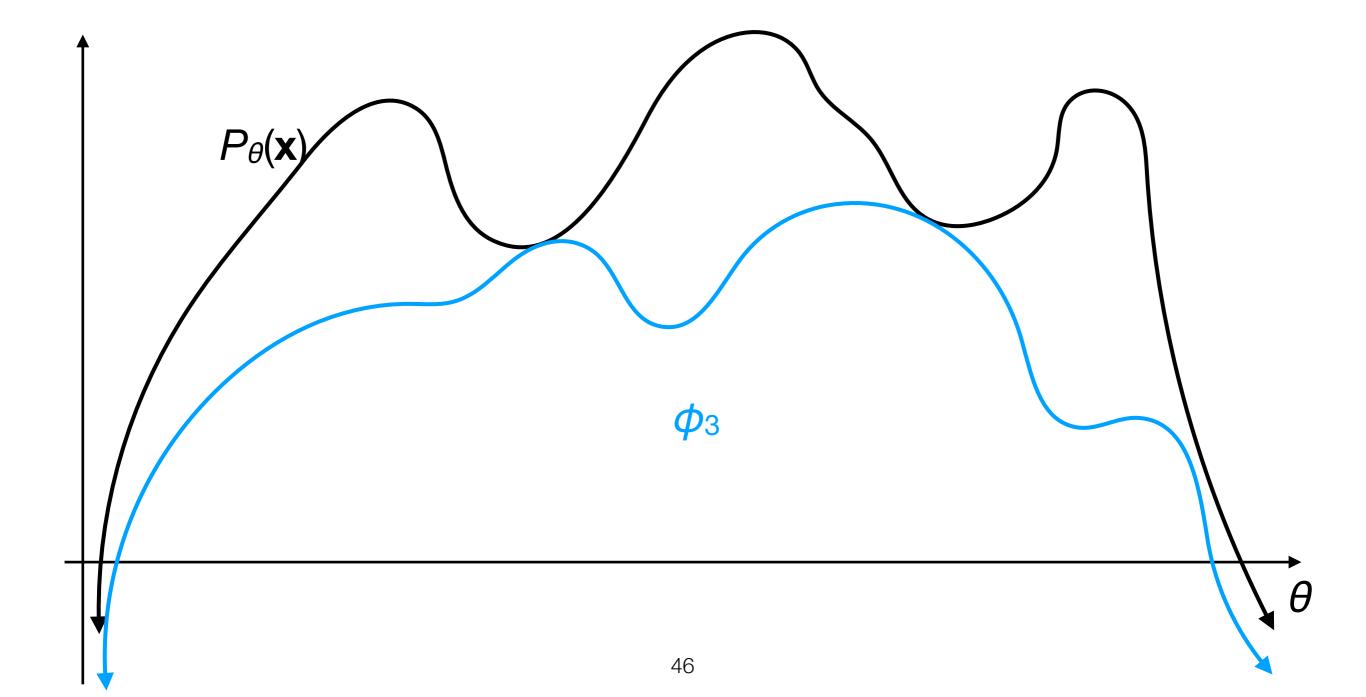
• We can approximately maximize  $P_{\theta}(\mathbf{x})$  w.r.t.  $\theta$  by maximizing the lower bound w.r.t.  $\theta$  and  $\phi$ .



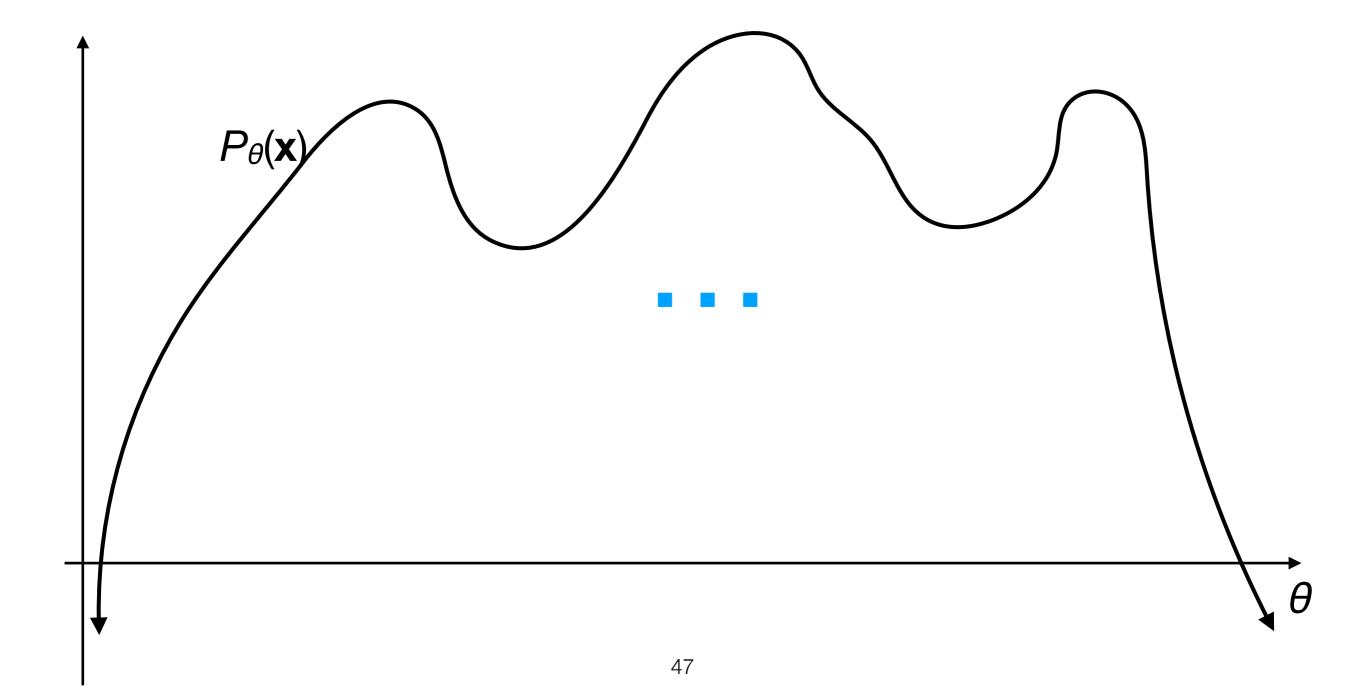
• By iteratively updating Q w.r.t.  $\phi$ , we can increase the upper bound (though it will never exceed  $P_{\theta}(\mathbf{x})$ ).



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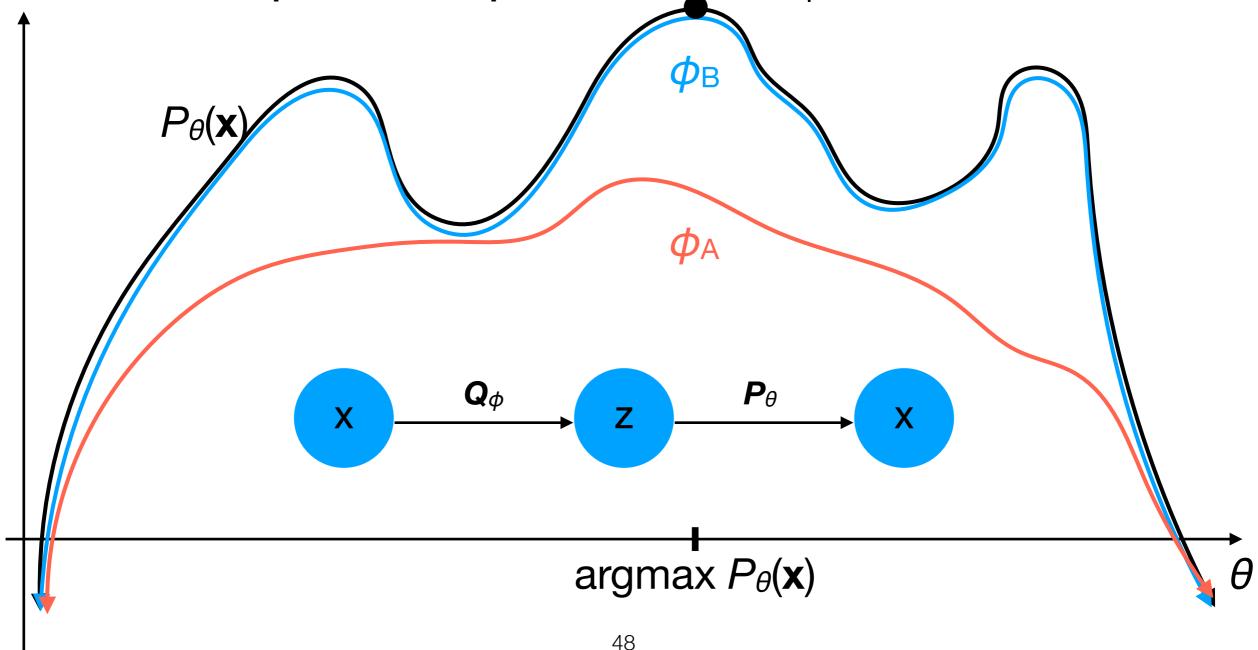
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### Solution

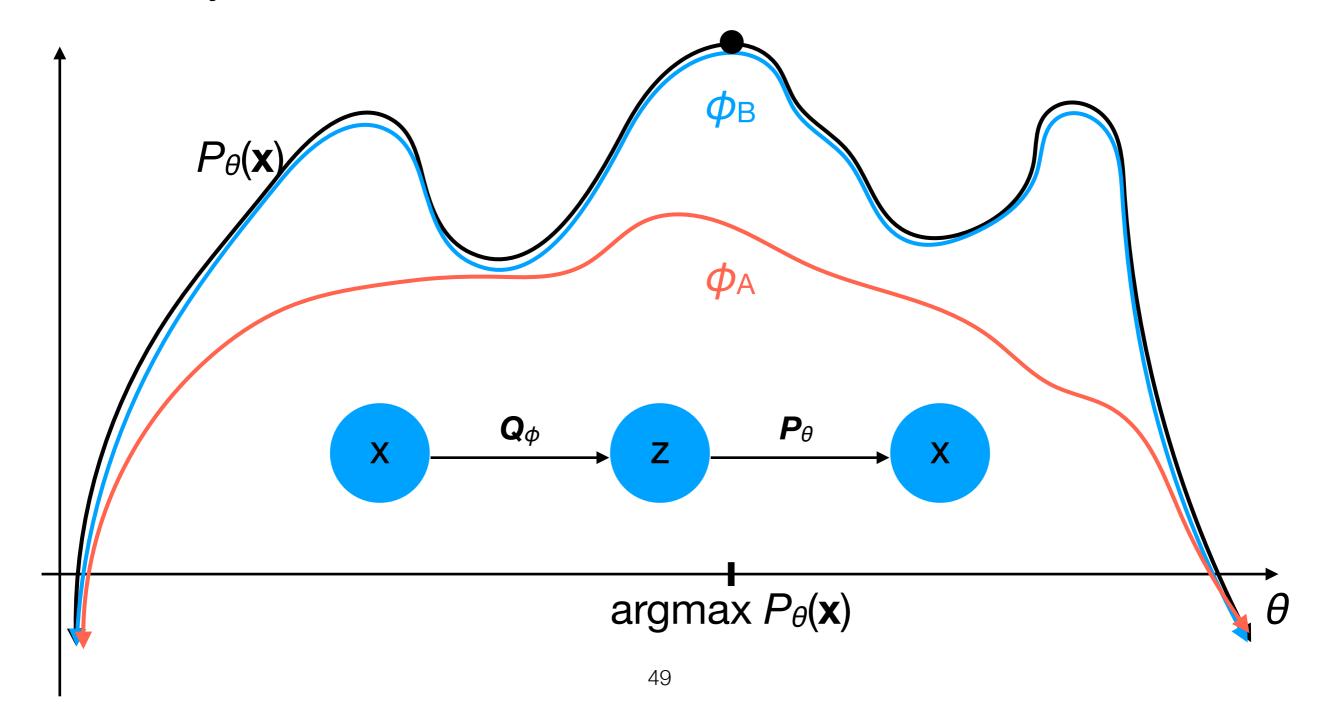
- However: if the approximation is "too tight", then Q(z | x) ≈ P(z) i.e., Q "ignores" x altogether and adheres "too much" to P(z).
- P thus receives no specific information about  $\mathbf{x}$  to reconstruct it with despite the tightness of the bound, SGD has no ability to find the "good" values for  $\theta$ .

This is called posterior collapse and is a common problem with VAEs.



#### Solution

•  $\phi_A$  is a looser lower bound, but it will likely yield a better estimate (via SGD) of  $argmax_\theta P_\theta(\mathbf{x})$  — which is what we really care about.



### **Avoiding Posterior Collapse**

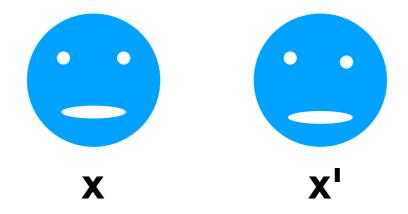
- It is common practice when training VAEs to weight (with hyperparameter  $\beta$ ) how much we care about the DL term versus the reconstruction term:
  - Modified ELBO:

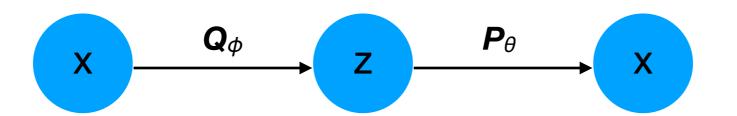
$$-\beta D_{\mathrm{KL}}(Q_{\phi}(\mathbf{z} \mid \mathbf{x}) \parallel P(\mathbf{z})) + \log P_{\theta}(\mathbf{x} \mid \mathbf{z})$$

- VAEs are known to produce blurry images. Why?
- Consider a decoder likelihood model  $P(\mathbf{x} \mid \mathbf{z}) = \mathcal{N}(\mu_{\mathbf{x}}, \mathbf{I})$  i.e., based on a latent  $\mathbf{z}$ , the mean  $\mu_{\mathbf{x}}$  of a Gaussian is chosen as the expected generated image.

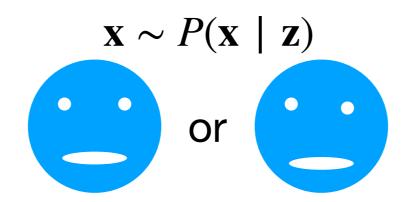
$$X \longrightarrow Q_{\phi} \longrightarrow Z \longrightarrow X$$

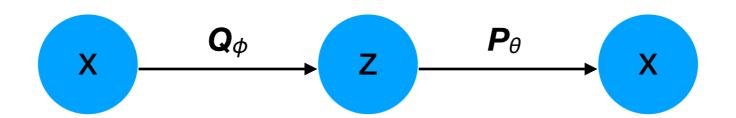
- Now, suppose two images x, x' are similar to each other and have identical latent codes z.
  - Why? Because in practice, it's difficult for latent z to perfectly encode all features of an image x.





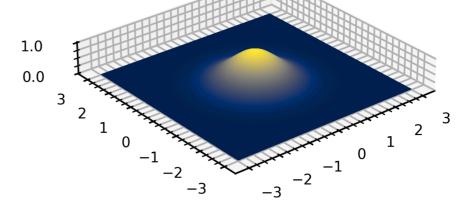
 Ideally, when sampling from P(x | z), we would obtain either of the two images, and they would both be "sharp" images.





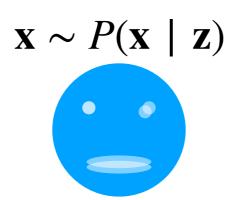
However, a Gaussian model

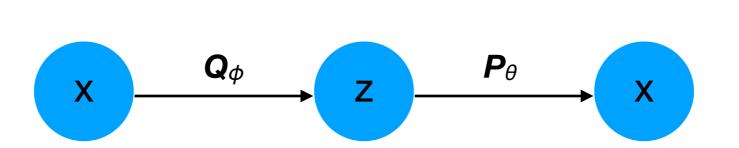
$$\mathcal{N}(\mu_{\mathbf{x}}, \mathbf{I}) \propto \exp\left(-\frac{1}{2}|\mathbf{x} - \mu_{\mathbf{x}}|^2\right)$$



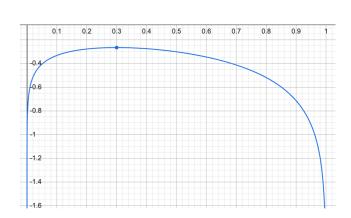
cannot express this — it is a unimodal distribution where likelihood shrinks quickly as  $\mathbf{x}$  deviates from the mean  $\mu_x$ .

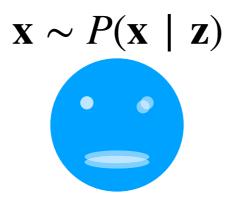
• For this reason, the decoder will maximize the likelihood over  $\{x, x'\}$  by picking  $\mu_x$  to be the *average* of the two images (see homework 1, part 4), creating blurry predictions.

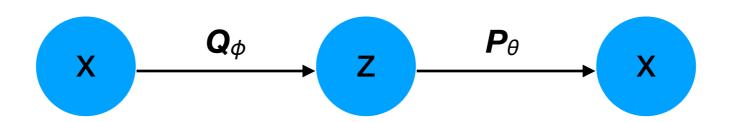




 The same problem exists for other likelihood models and reconstruction losses as well, e.g., binary cross-entropy.







## Group exercise

- Please do not use ChatGPT (or another Al tool) on this exercise.
- Download vae exercise.py from Canvas->Files.
- Answer the following questions:
  - 1. Where/what are all the bugs in the code?
  - 2. Which lines (which might not be contiguous!) of code implement the expectation  $\mathbb{E}_{Q(\mathbf{z} \mid \mathbf{x})}[P(\mathbf{x} \mid \mathbf{z})]$ , and how many samples is the expectation calculated over?
  - 3. Which lines (which might not be contiguous!) of code implement the KL divergence? Where are the inputs to the KL term calculated, and how do they relate to the formula in the slides?
  - 4. What is the dimension *d* of the code **z**?
  - 5. How many NN linear layers are traversed in the encoder to process each  $\mathbf{x}$  to produce the mean of  $P(\mathbf{z} \mid \mathbf{x})$ ?
  - 6. In terms of the VAE definition from the slides, what probability distribution does VAE.reparameterize() sample from?

## Group exercise

Prior dist. over latent code z

$$P(\mathbf{z}) = \mathcal{N}(\mathbf{0}, \mathbf{I})$$

Output of encoder Q:

$$(\mu^{(i)}, \sigma^{(i)^2}) = Q_{\phi}(\mathbf{z}^{(i)} \mid \mathbf{x}^{(i)}), \ \forall i$$

**ELBO**:

$$-D_{\mathrm{KL}}(Q_{\phi}(\mathbf{z} \mid \mathbf{x}) \parallel P(\mathbf{z})) + \mathbb{E}_{Q_{\phi}}[\log P_{\theta}(\mathbf{x} \mid \mathbf{z})]$$

KL divergence between two diagonal Gaussians:

$$D_{\text{KL}}(Q(\mathbf{z}) \parallel P(\mathbf{z})) = -\frac{1}{2} \sum_{j=1}^{m} (1 + \log(\sigma_j^2) - \mu_j^2 - \sigma_j^2)$$

