香港科技大學
THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY

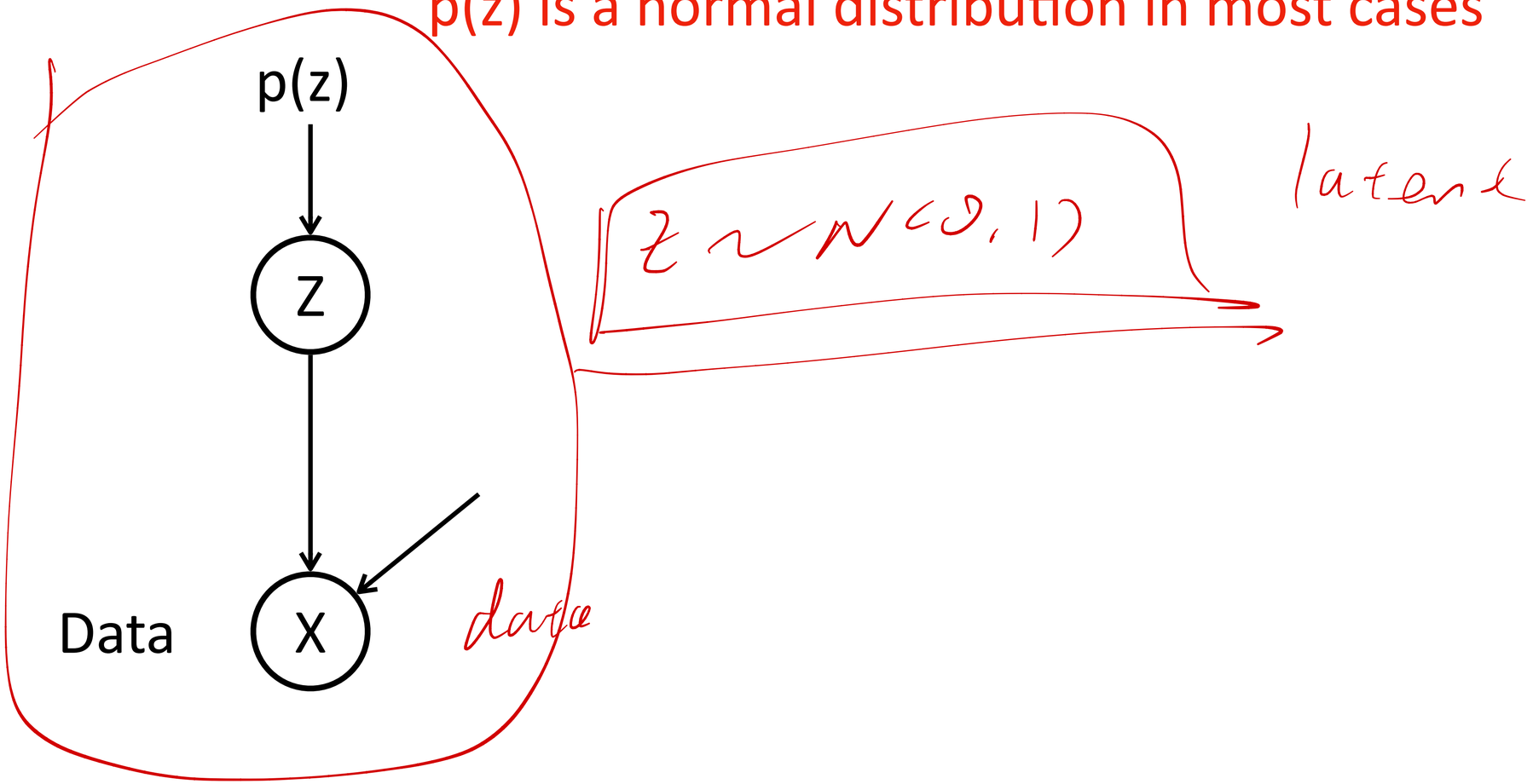
COMP 5212
Machine Learning
Lecture 14

Variational Autoencoders, Hidden Markov Models

Junxian He
Apr 2, 2026

Recap: The VAE Model

p(z) is a normal distribution in most cases



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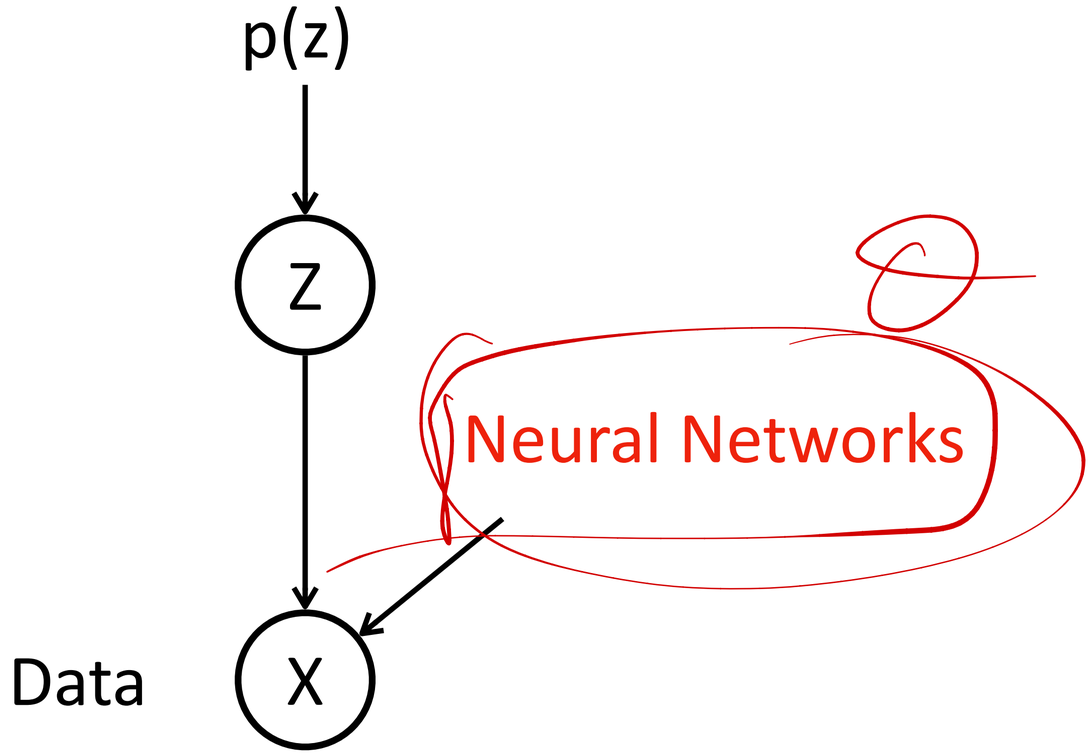

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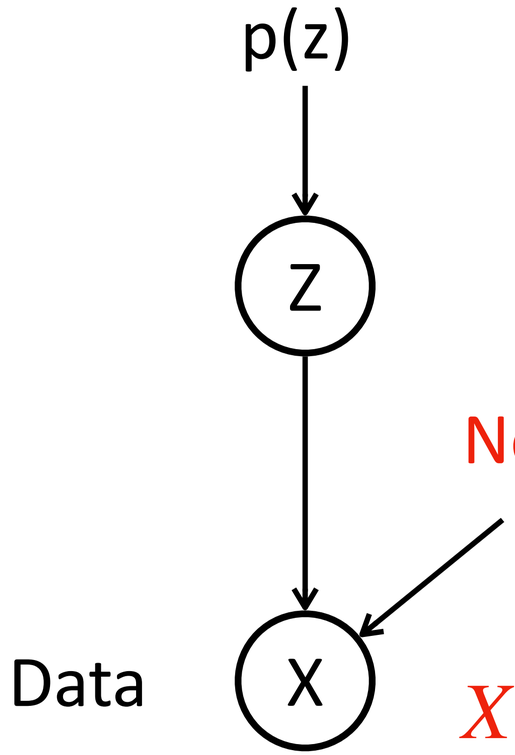

Neural Networks

$x \sim N(\mu = f(z;\theta), I)$

$f(z;\theta)$

$X \sim P(x, f(z;\theta))$

N
Categorical

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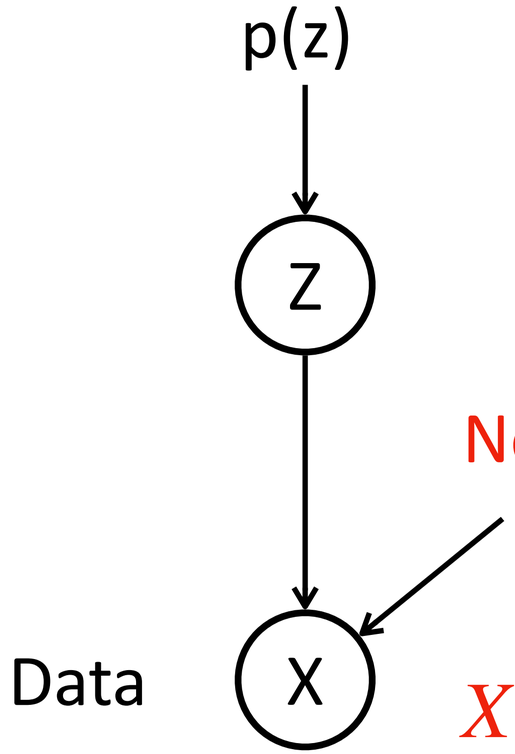
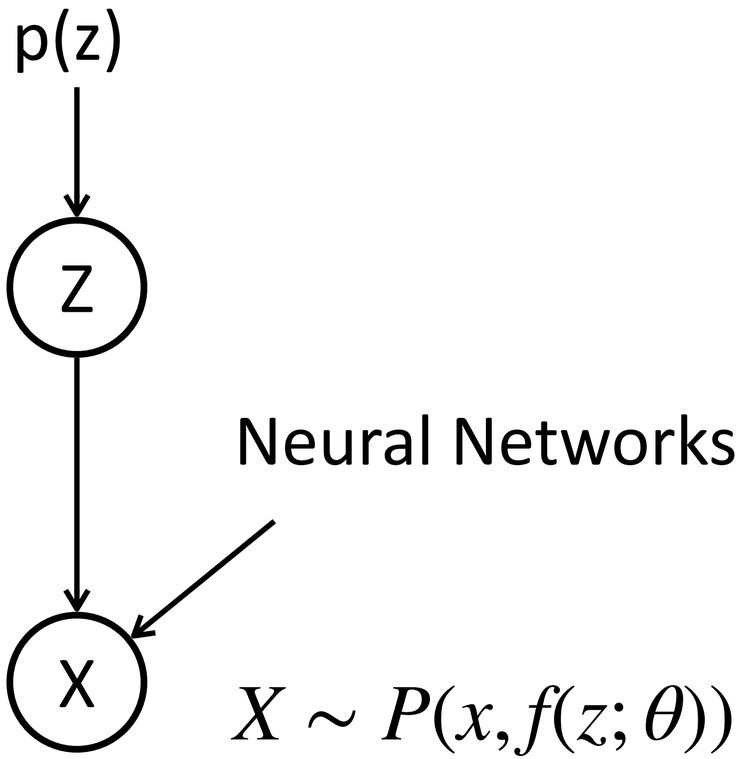


Neural Networks

$$X \sim P(x, f(z;\theta))$$

f is a neural network taking Z as input

Training



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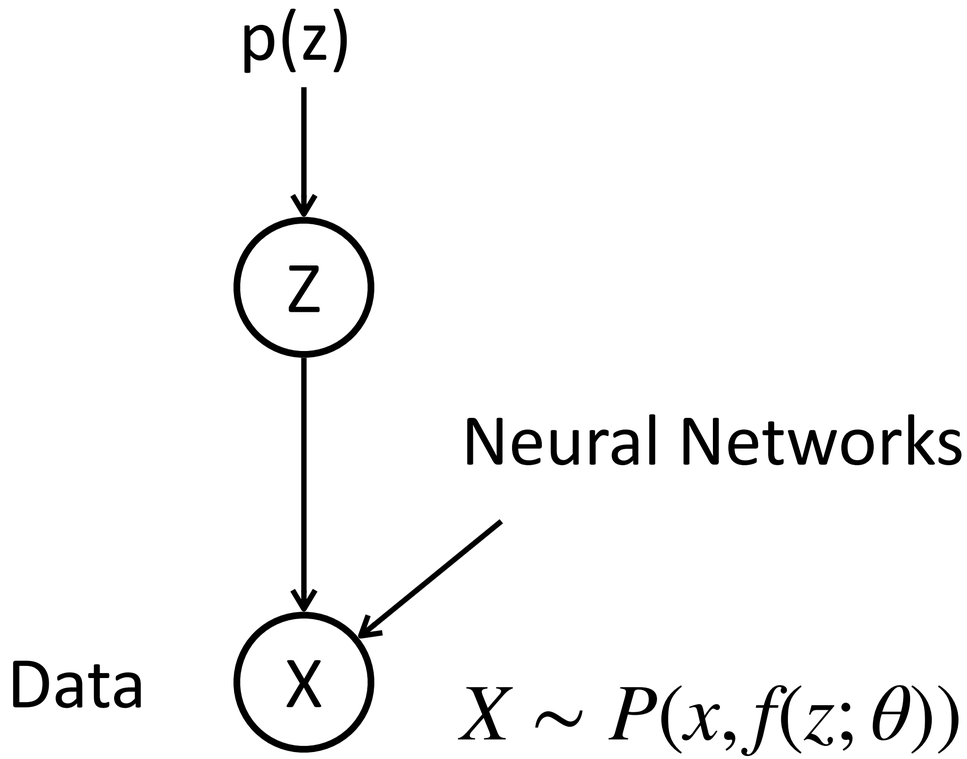
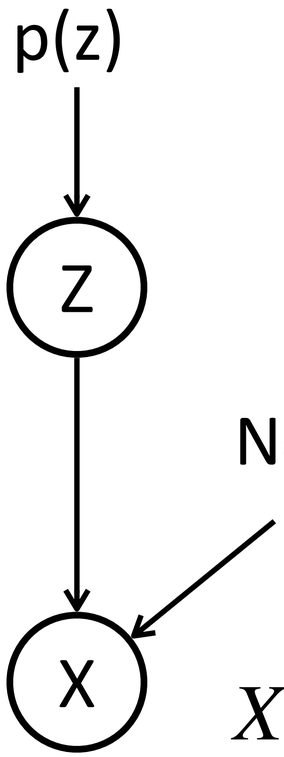


How to train the model? Can we do MLE?

Training



Neural Networks

Data

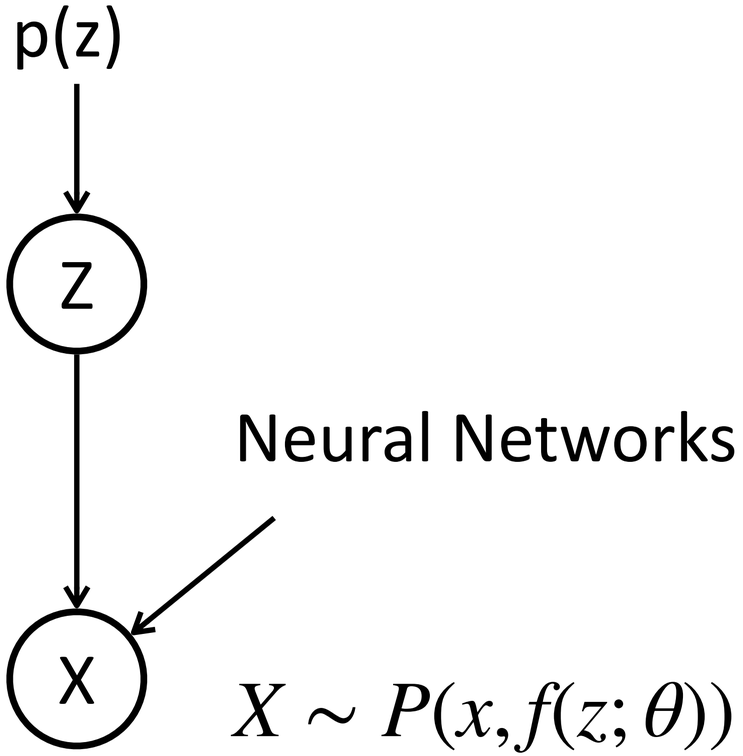
$$X \sim P(x, f(z;\theta))$$

How to train the model? Can we do MLE?

Intractable P(X), EM algorithm?

$$\int_z P(x,z)\,dz$$

Let's try EM



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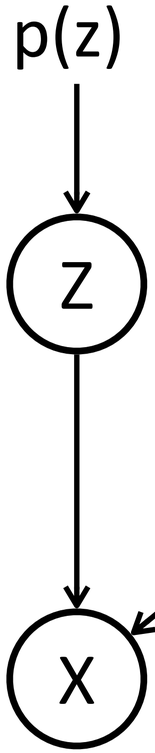


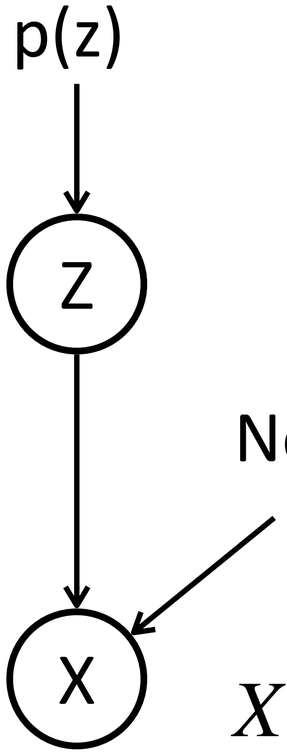
Neural Networks

$$X \sim P(x, f(z;\theta))$$

E-Step: compute P(z|x)

$$Q(z) = P(z \mid x) \propto P(z)P(x \mid z)$$

Let's try EM



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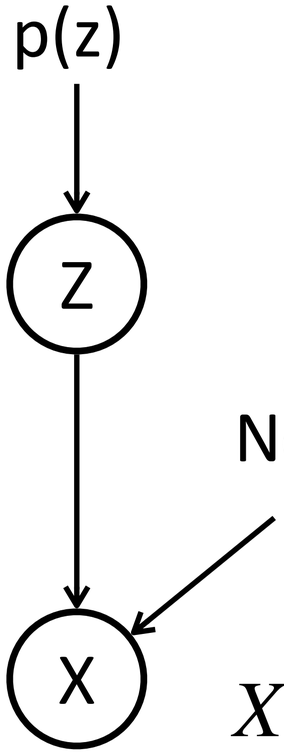

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M-Step: the ELBO objective

$$\text{argmax}_\theta \sum_z Q(z) \log p(x, z; \theta) = \text{argmax}_\theta \mathbb{E}_{z \sim Q(z)} \log p(x, z; \theta)$$

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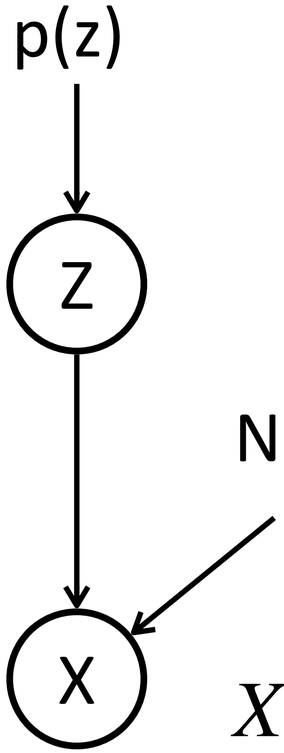

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In most cases, we cannot do the sum, and cannot easily sample from Q(z) either

Approximate Posterior

We need an easy-to-sample distribution to approximate $P(z|x)$

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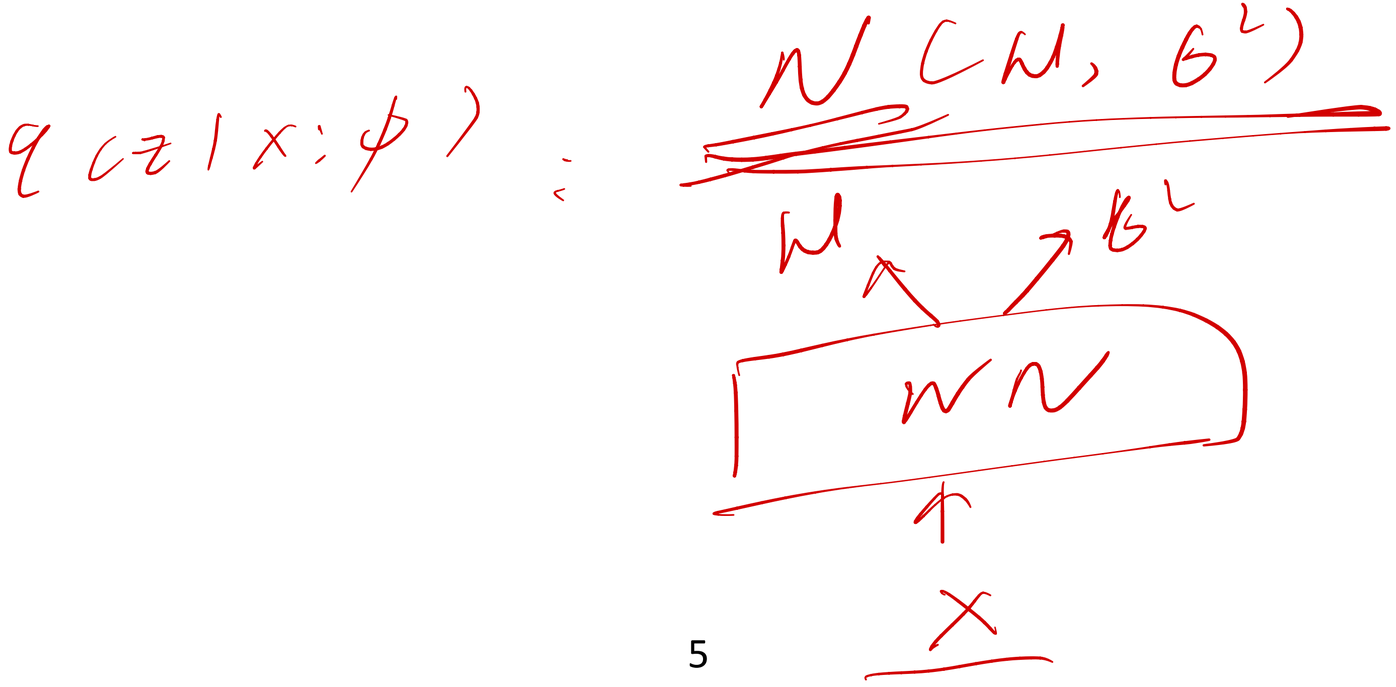

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$q(z|x;\phi)$ to approximate $p(z|x;\theta)$ Why conditioned on x?

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How to train $q(z|x;\phi)$, what would be the loss to find ϕ?

E step: $q(z|x;\phi) \longrightarrow P(z|x;\theta)$

Recap: ELBO

$$\mathrm{ELBO}(x; Q, \theta) = \sum_z Q(z) \log \frac{p(x, z; \theta)}{Q(z)}$$

What is $\mathrm{argmax}_{Q(z)} \mathrm{ELBO}(x; Q, \theta)$?

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ELBO is maximized when Q(z) is equal to p(z|x)

$Q(z) = p(z|x)$

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Therefore, we can approximate the true posterior by maximizing ELBO:

$$\text{argmax}_\phi \sum_z q(z|x;\phi) \log \frac{p(x, z; \theta)}{q(z|x;\phi)}$$

constant, not depend Q

$$ELBO = \log P(x;\theta) - KL(Q \| P(z|x;\theta))$$

$$\arg\max_{Q} ELBO = \arg\min_{Q} KL(Q \| P(z|x;\theta))$$

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Variational Inference

Training VAEs

E-Step:

$$\text{argmax}_{\phi} \sum_{z} q(z \mid x; \phi) \log \frac{p(x, z; \theta)}{q(z \mid x; \phi)}$$

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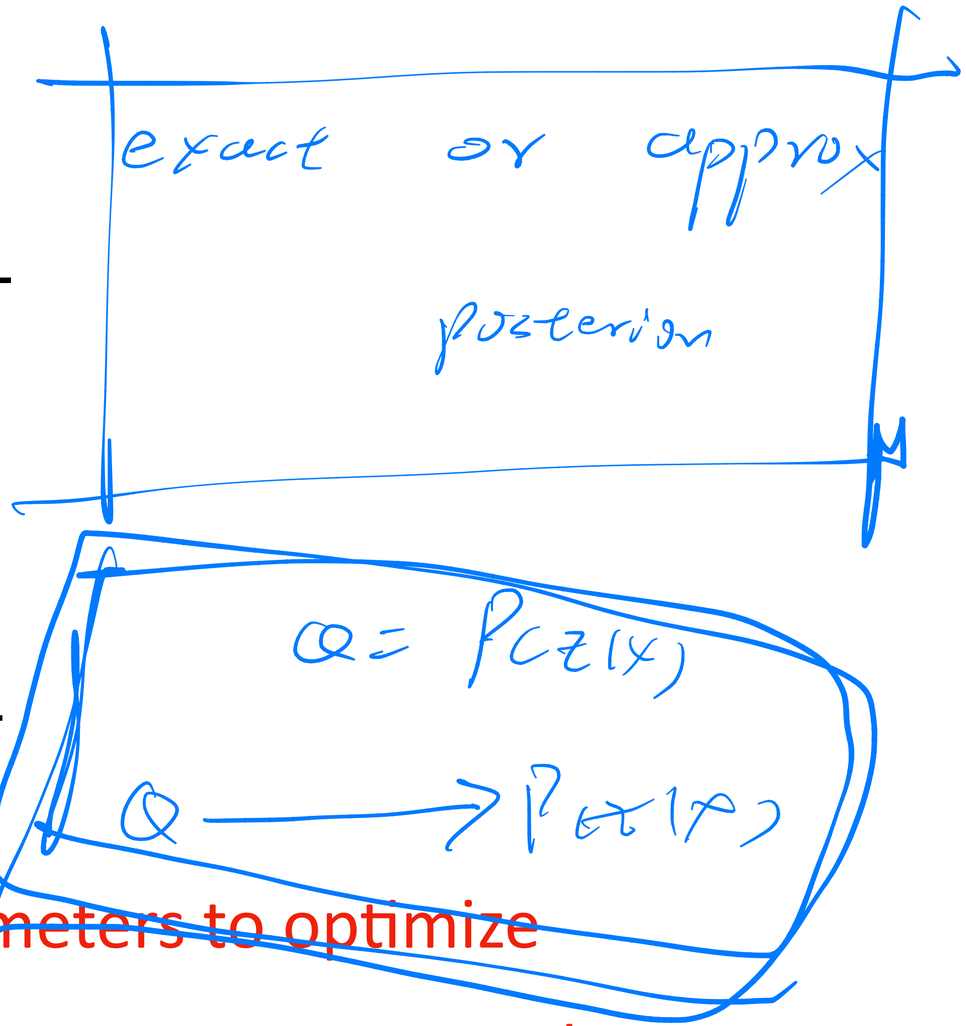

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Because we use approximate rather than exact posterior, it is also called Variational EM

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We use MC sampling to approximate expectation and use gradient descent to optimize θ

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Can we do gradient descent over ϕ?

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First, we cannot do sum, but we can sample z_i from $q(z \mid x; \phi)$, which depends on ϕ, how do we propagate gradients to ϕ?

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Can you verify z in this equation is Gaussian?

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For every gradient step (assuming batch size=1):

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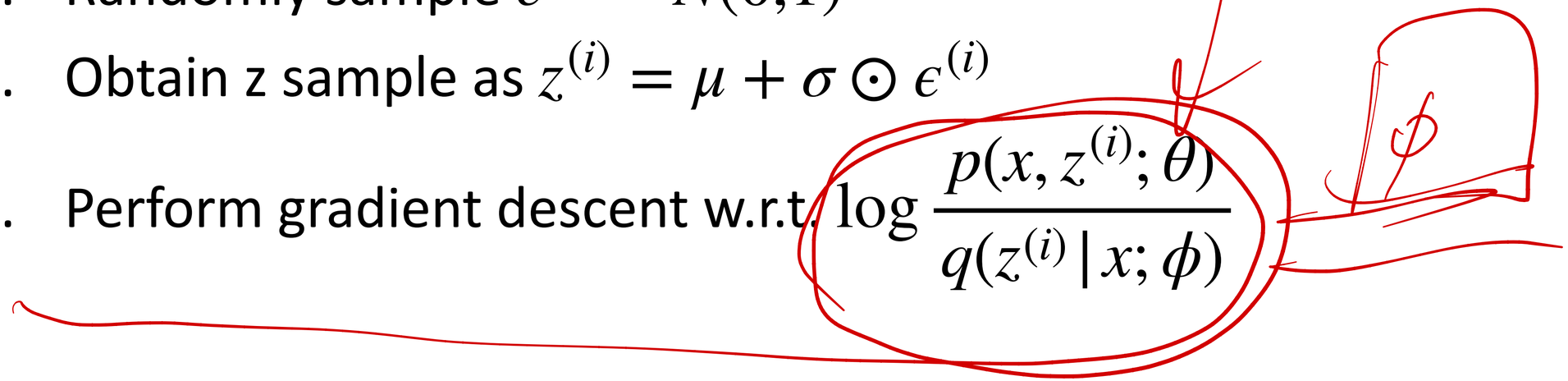

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We can now propagate gradients from z to ϕ

ELBO

$$\sum_{z} q(z \mid x; \phi) \log \frac{p(x, z; \theta)}{q(z \mid x; \phi)} = \mathbb{E}_{z \sim q_\phi(z|x)}[\log p_\theta(x, z) - \log q_\phi(z \mid x)]$$

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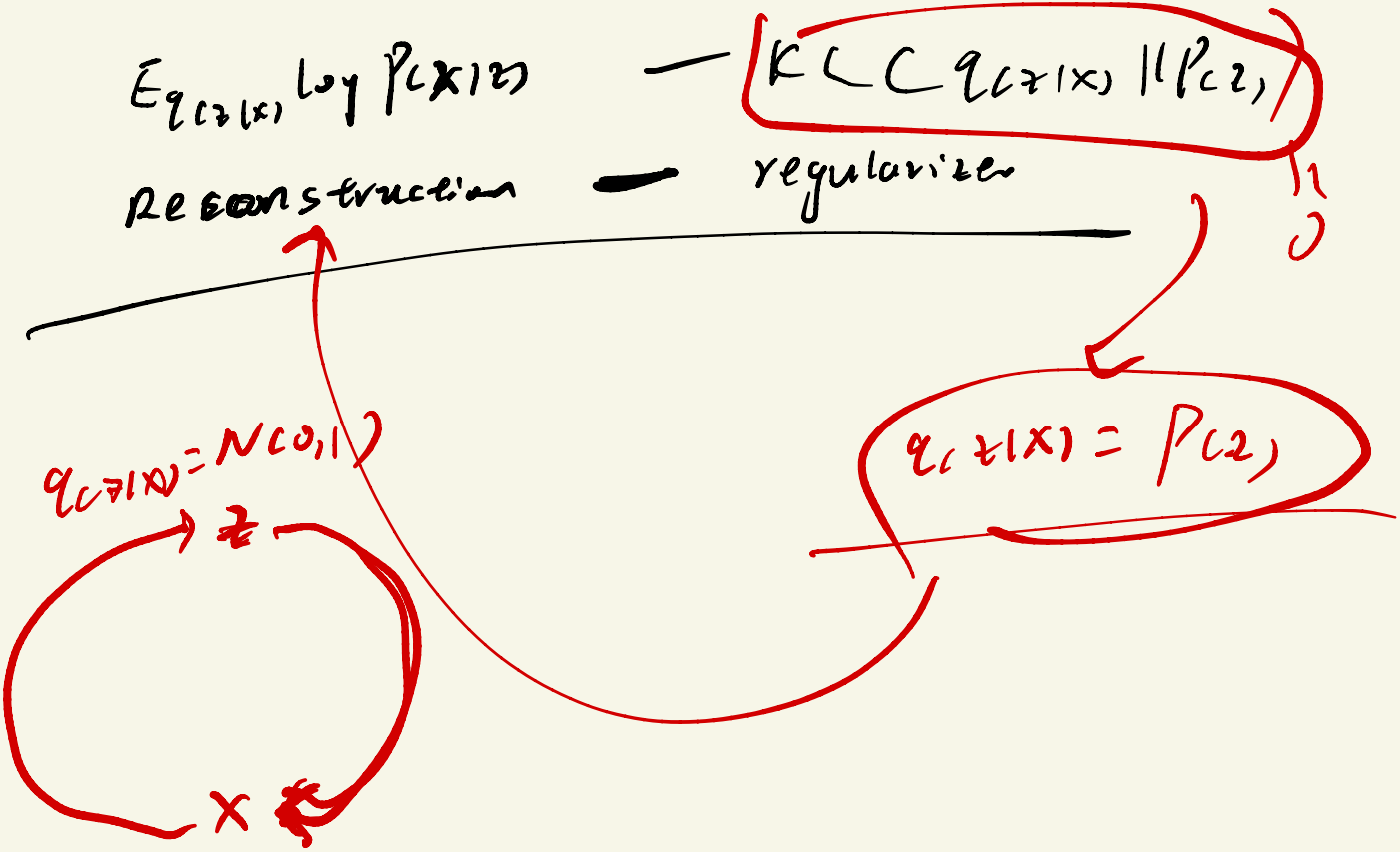
ELBO is implemented with the following form:

$$\underbrace{\mathbb{E}_{\mathbf{z} \sim q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})}[\log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})]}_{\text{Reconstruction Loss}} - \underbrace{D_{\mathrm{KL}}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z}))}_{\text{KL Regularizer}}$$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Reconstruction
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z
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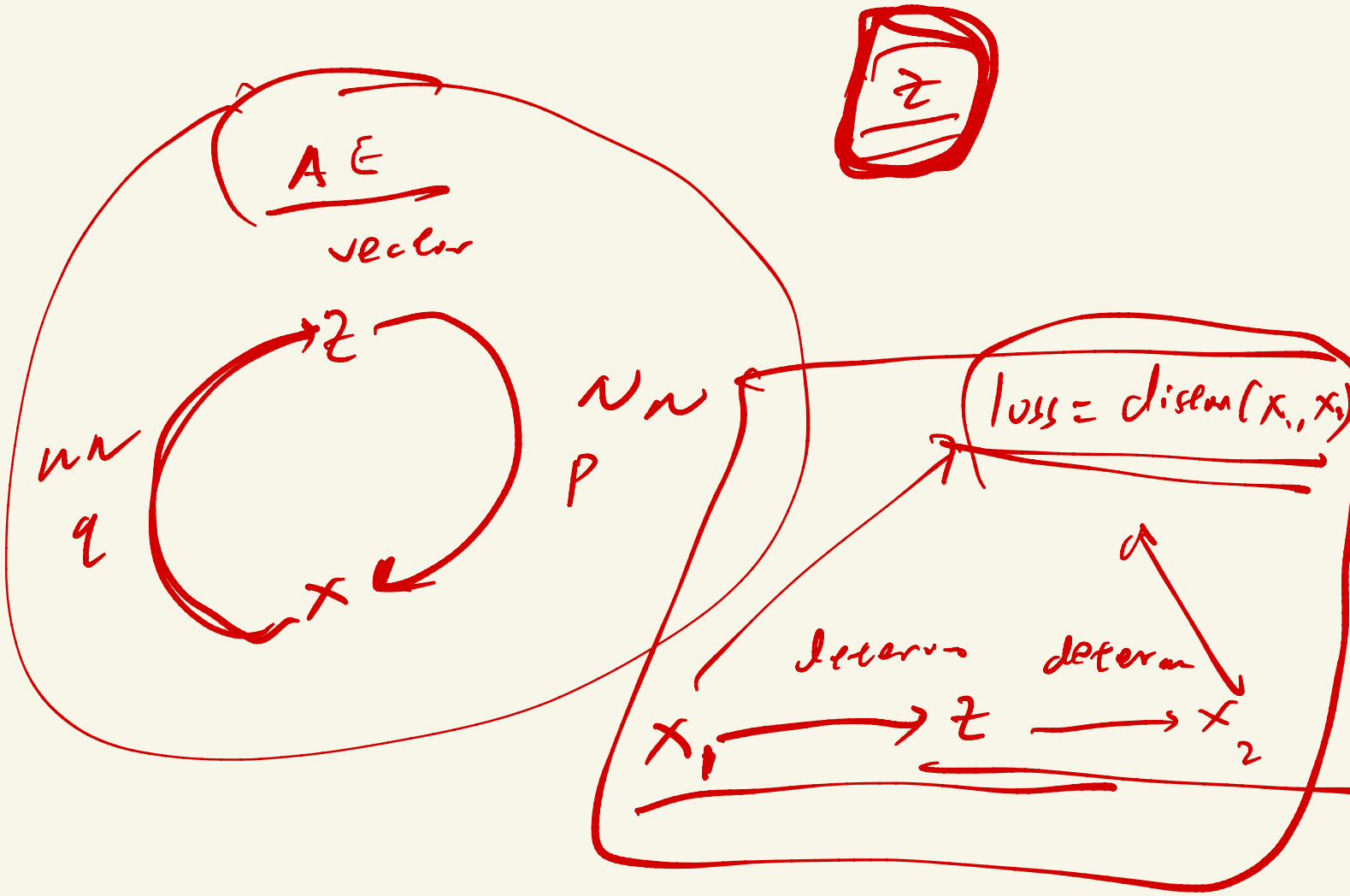
Autoencoder


z
AE
vector
z
NN
q
NN
p
x
loss = distance(x1, x2)
x1
deterministic
z
deterministic
x2

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Autoencoder Loss

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Autoencoder Loss

q(z|x) and p(z) are both Gaussian, there is a closed-form for this

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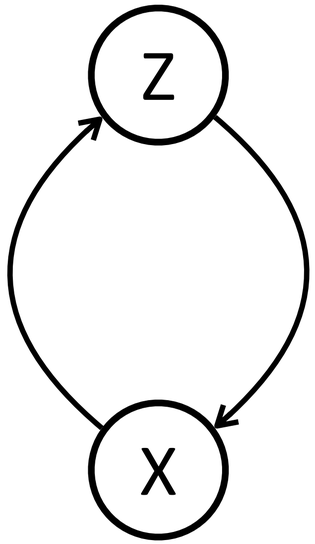

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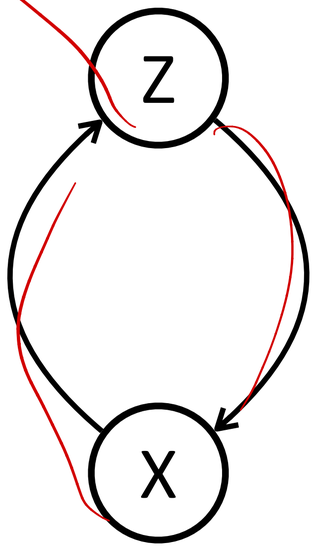

$$ELBO = \log P(x;\theta) - KL(q(z|x) \,||\, p(z|x))$$

This is why it is called variational "autoencoder"

ELBO

$$D_{\mathrm{KL}}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})||p(\mathbf{z}))$$

ELBO

$$D_{\mathrm{KL}}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})\|p(\mathbf{z}))$$

$$\int q_{\boldsymbol{\theta}}(\mathbf{z}) \log p(\mathbf{z})\, d\mathbf{z} = \int \mathcal{N}(\mathbf{z}; \boldsymbol{\mu}, \boldsymbol{\sigma}^2) \log \mathcal{N}(\mathbf{z}; \mathbf{0}, \mathbf{I})\, d\mathbf{z}$$

$$= -\frac{J}{2}\log(2\pi) - \frac{1}{2}\sum_{j=1}^{J}(\mu_j^2 + \sigma_j^2)$$

J is the dimensionality of z

ELBO

$$D_{\mathrm{KL}}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})||p(\mathbf{z}))$$

$$\int q_{\boldsymbol{\theta}}(\mathbf{z}) \log p(\mathbf{z})\, d\mathbf{z} = \int \mathcal{N}(\mathbf{z}; \boldsymbol{\mu}, \boldsymbol{\sigma}^2) \log \mathcal{N}(\mathbf{z}; \mathbf{0}, \mathbf{I})\, d\mathbf{z}$$

$$= -\frac{J}{2}\log(2\pi) - \frac{1}{2}\sum_{j=1}^{J}(\mu_j^2 + \sigma_j^2)$$

J is the dimensionality of z

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$$-D_{KL}((q_{\boldsymbol{\phi}}(\mathbf{z})||p_{\boldsymbol{\theta}}(\mathbf{z})) = \int q_{\boldsymbol{\theta}}(\mathbf{z}) \left(\log p_{\boldsymbol{\theta}}(\mathbf{z}) - \log q_{\boldsymbol{\theta}}(\mathbf{z})\right)\, d\mathbf{z}$$

$$= \frac{1}{2}\sum_{j=1}^{J}\left(1 + \log((\sigma_j)^2) - (\mu_j)^2 - (\sigma_j)^2\right)$$

Training VAEs

E-Step:

$$\text{argmax}_{\phi} \underbrace{\mathbb{E}_{\mathbf{z}\sim q_{\phi}(\mathbf{z}|\mathbf{x})}[\log p_{\theta}(\mathbf{x}|\mathbf{z})]}_{\text{Reconstruction Loss}} - \underbrace{D_{\text{KL}}(q_{\phi}(\mathbf{z}|\mathbf{x})\|p(\mathbf{z}))}_{\text{KL Regularizer}}$$

M-Step:

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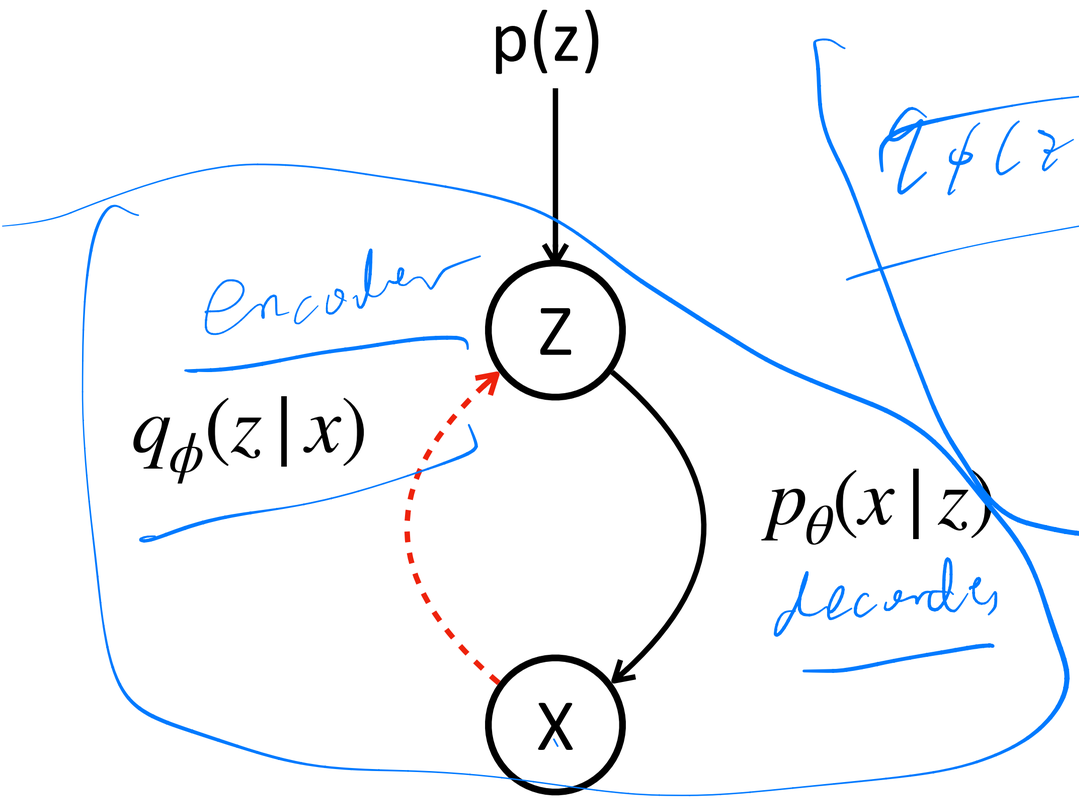
Intuitively we hope to approximate p(z|x) with q(z|x) accurately in the E-step, to approximate the true EM algorithm

Review VAE



ELBO Loss

ϕ θ

$q_\phi(z|x)$ NN Inference Net

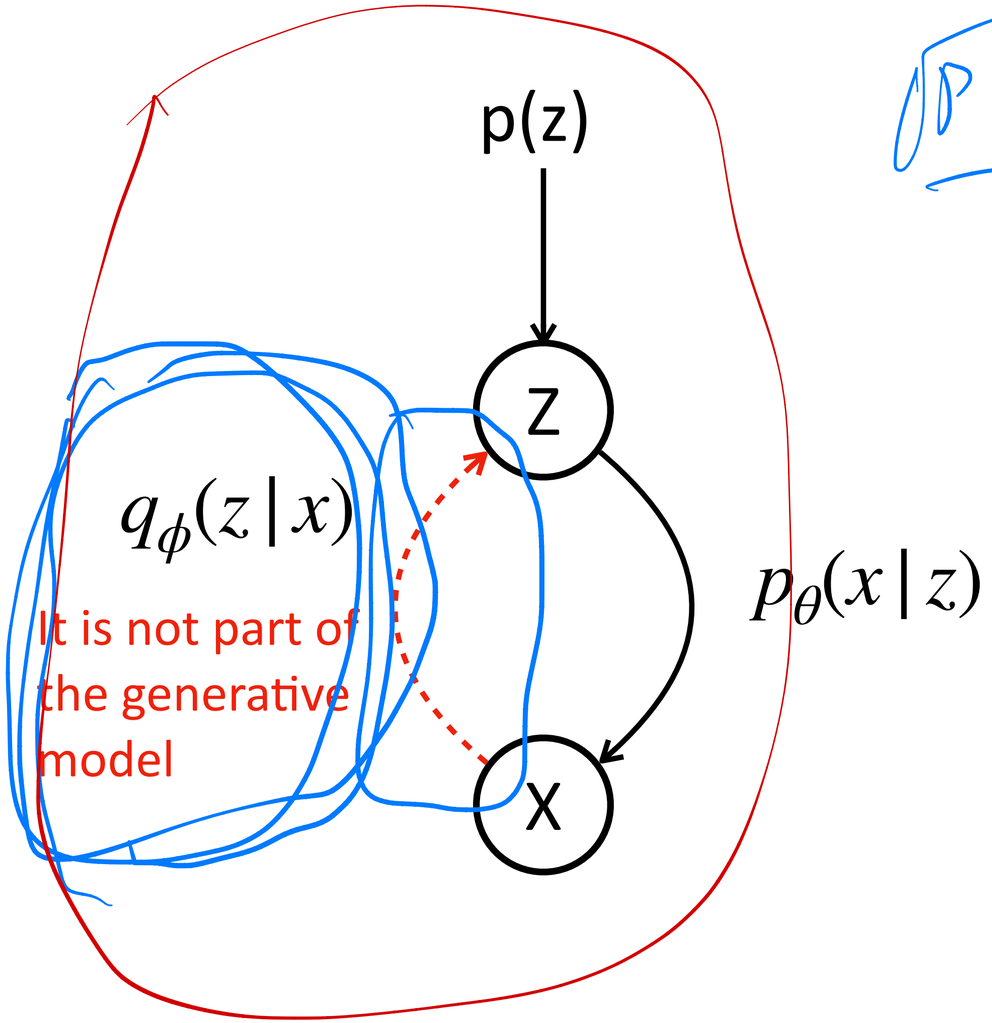
$p_\theta(x|z)$ NN generative net

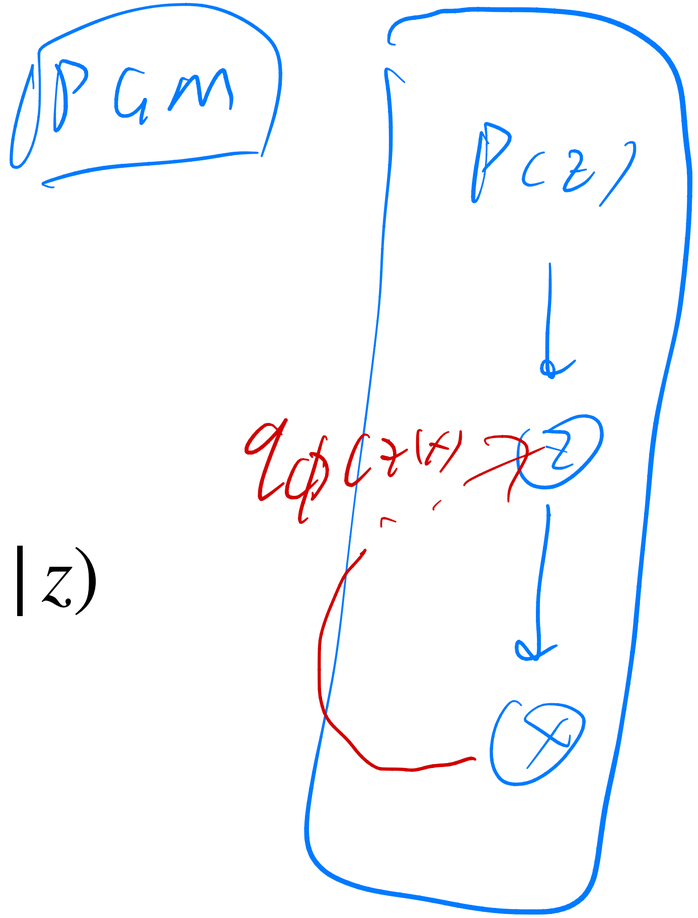
Encoder

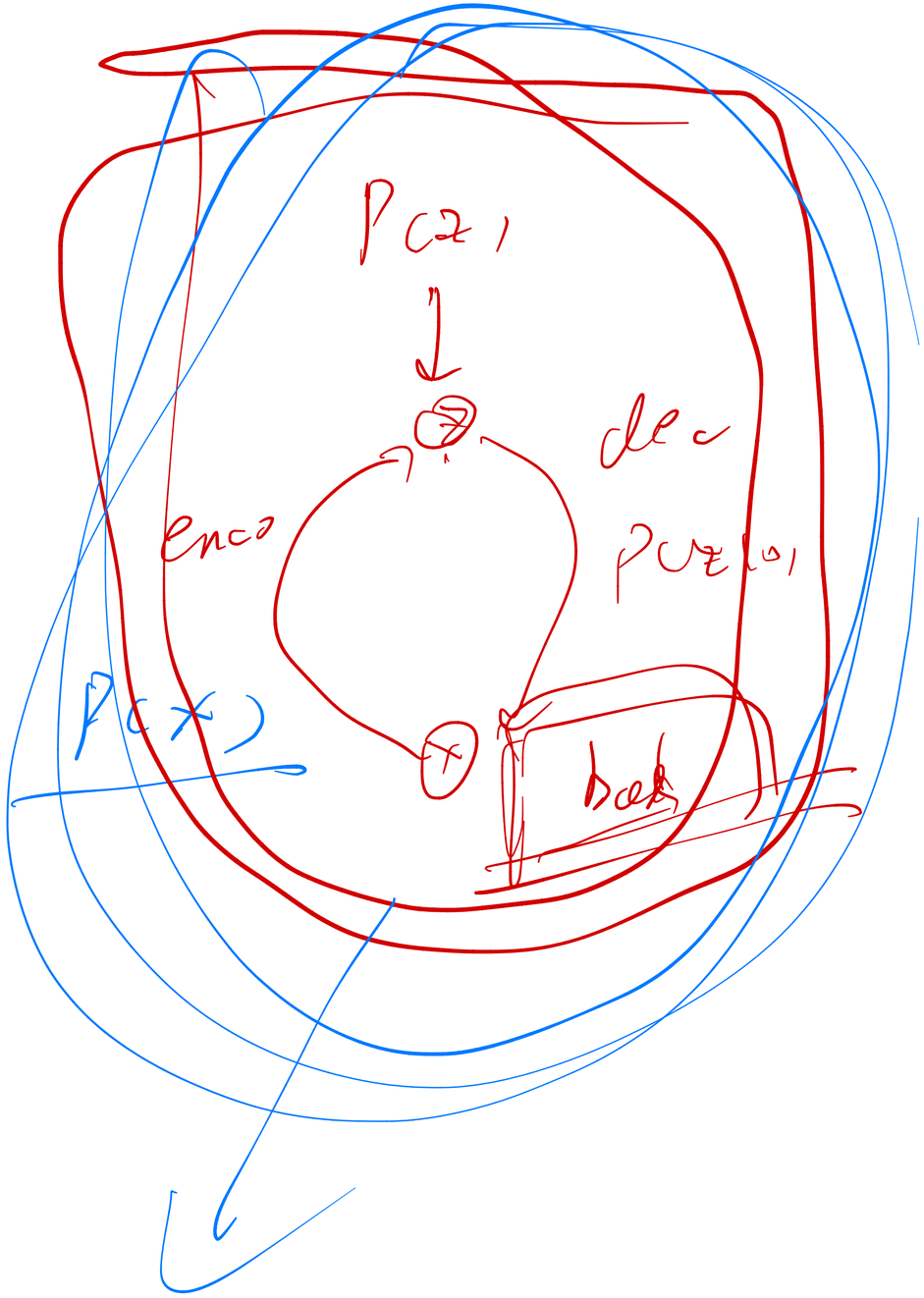
decoder

VAE model

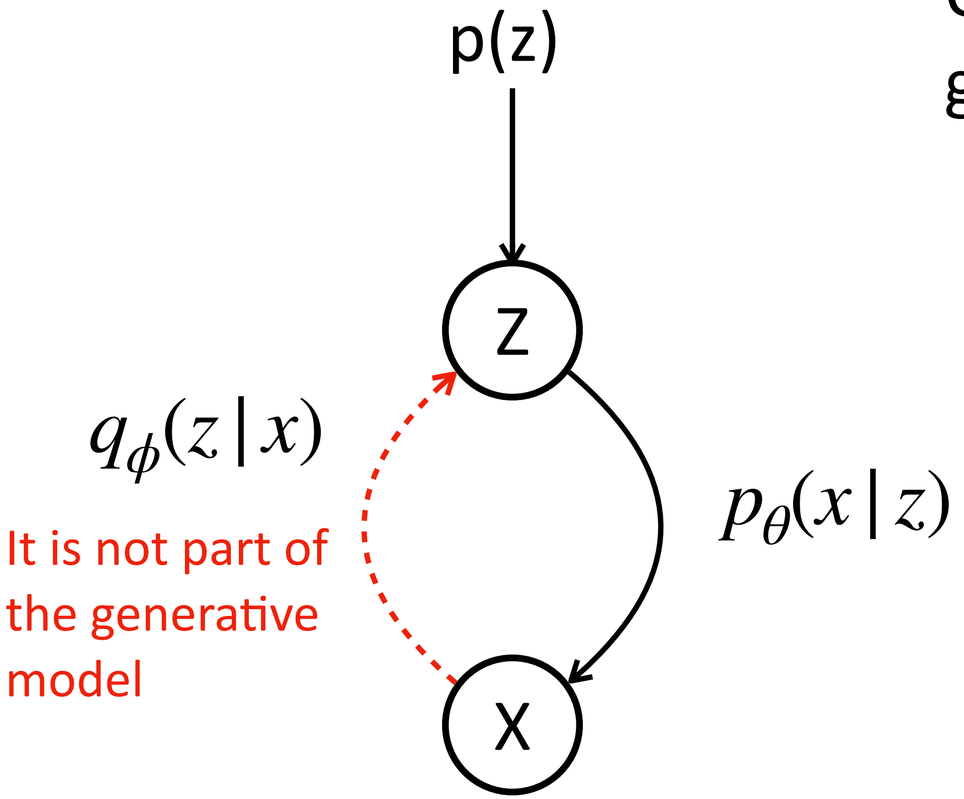
Review VAE


p(z)
z
x
$q_\phi(z \mid x)$
$p_\theta(x \mid z)$
It is not part of the generative model


PGM
p(z)
$q_\phi(z \mid x)$
z
x

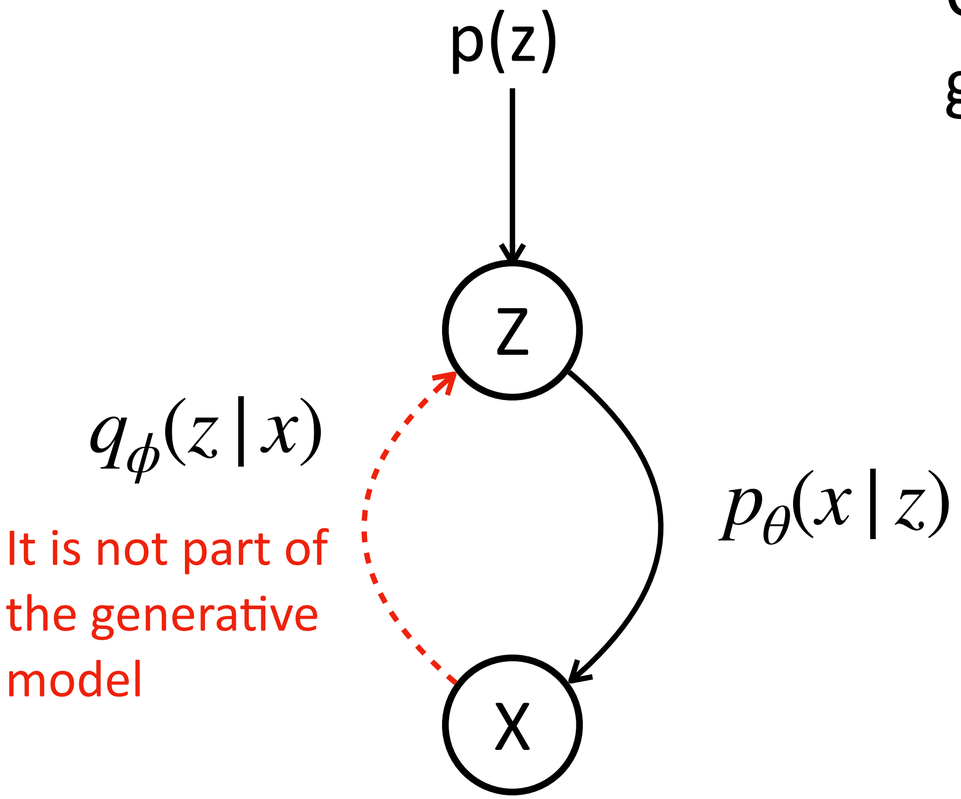

p(z)
enco
dec
p(x|z)
p(x)
x
bce

Review VAE



Only the right (black) part defines the generative model, and the distribution

Review VAE



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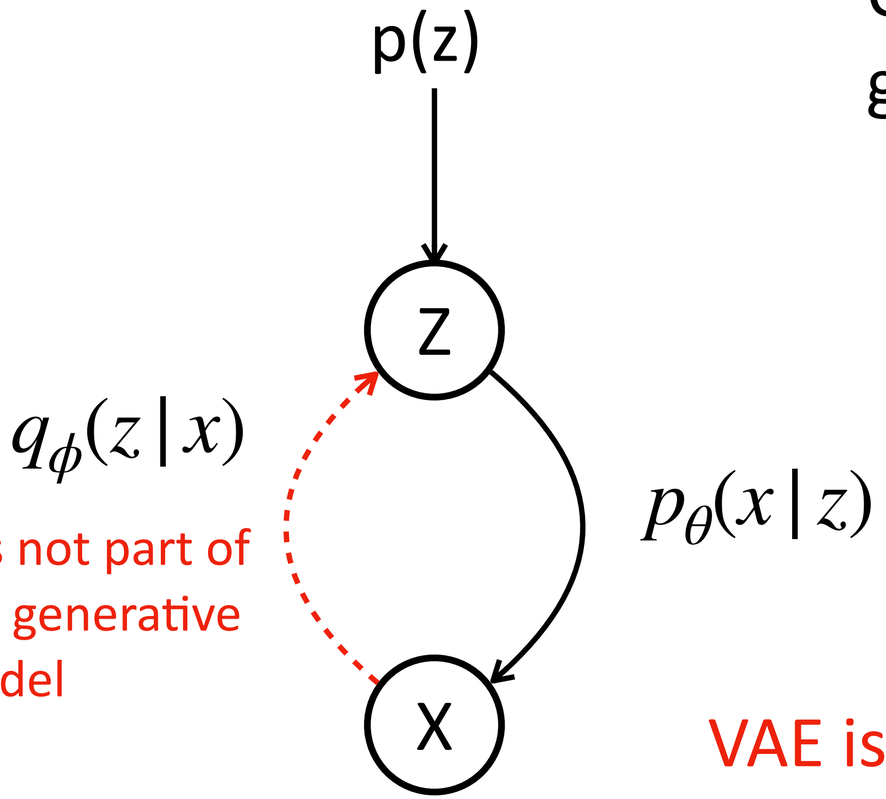
$p_\theta(x \mid z)$: generative network/decoder

$q_\phi(z \mid x)$: inference network/encoder

Review VAE



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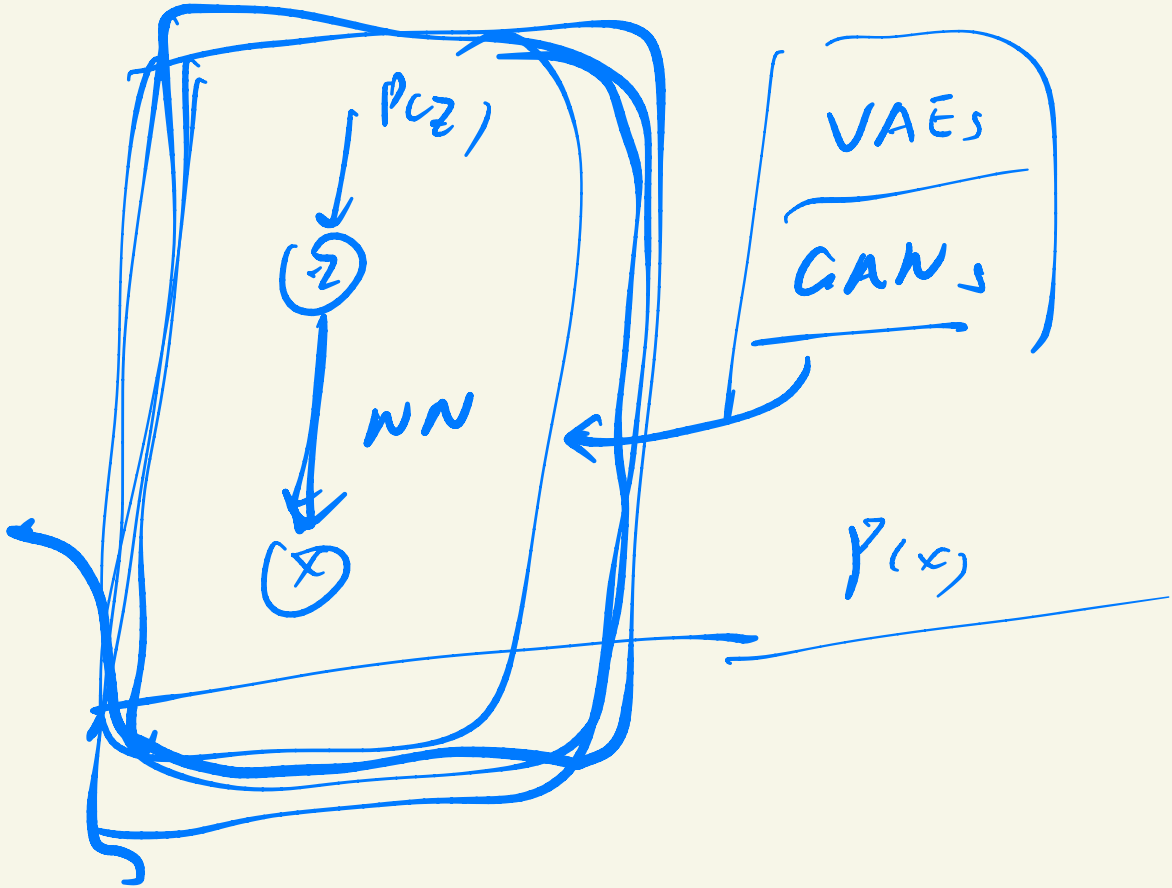
VAE: { model + traing method

VAE is a name to represent both the model p(x) and the inference network that is used to train the model, but do not confuse them together


P(z)
z
NN
x
VAEs
GANs
P(x)

Training VAEs

Algorithm 1 Minibatch version of the Auto-Encoding VB (AEVB) algorithm. Either of the two SGVB estimators in section 2.3 can be used. We use settings $M = 100$ and $L = 1$ in experiments.

$\boldsymbol{\theta}, \boldsymbol{\phi} \leftarrow$ Initialize parameters
repeat
  $\mathbf{X}^M \leftarrow$ Random minibatch of M datapoints (drawn from full dataset)
  $\boldsymbol{\epsilon} \leftarrow$ Random samples from noise distribution $p(\boldsymbol{\epsilon})$
  $\mathbf{g} \leftarrow \nabla_{\boldsymbol{\theta},\boldsymbol{\phi}} \widetilde{\mathcal{L}}^M(\boldsymbol{\theta}, \boldsymbol{\phi}; \mathbf{X}^M, \boldsymbol{\epsilon})$ (Gradients of minibatch estimator (8))
  $\boldsymbol{\theta}, \boldsymbol{\phi} \leftarrow$ Update parameters using gradients $\mathbf{g}$ (e.g. SGD or Adagrad [DHS10])
until convergence of parameters $(\boldsymbol{\theta}, \boldsymbol{\phi})$
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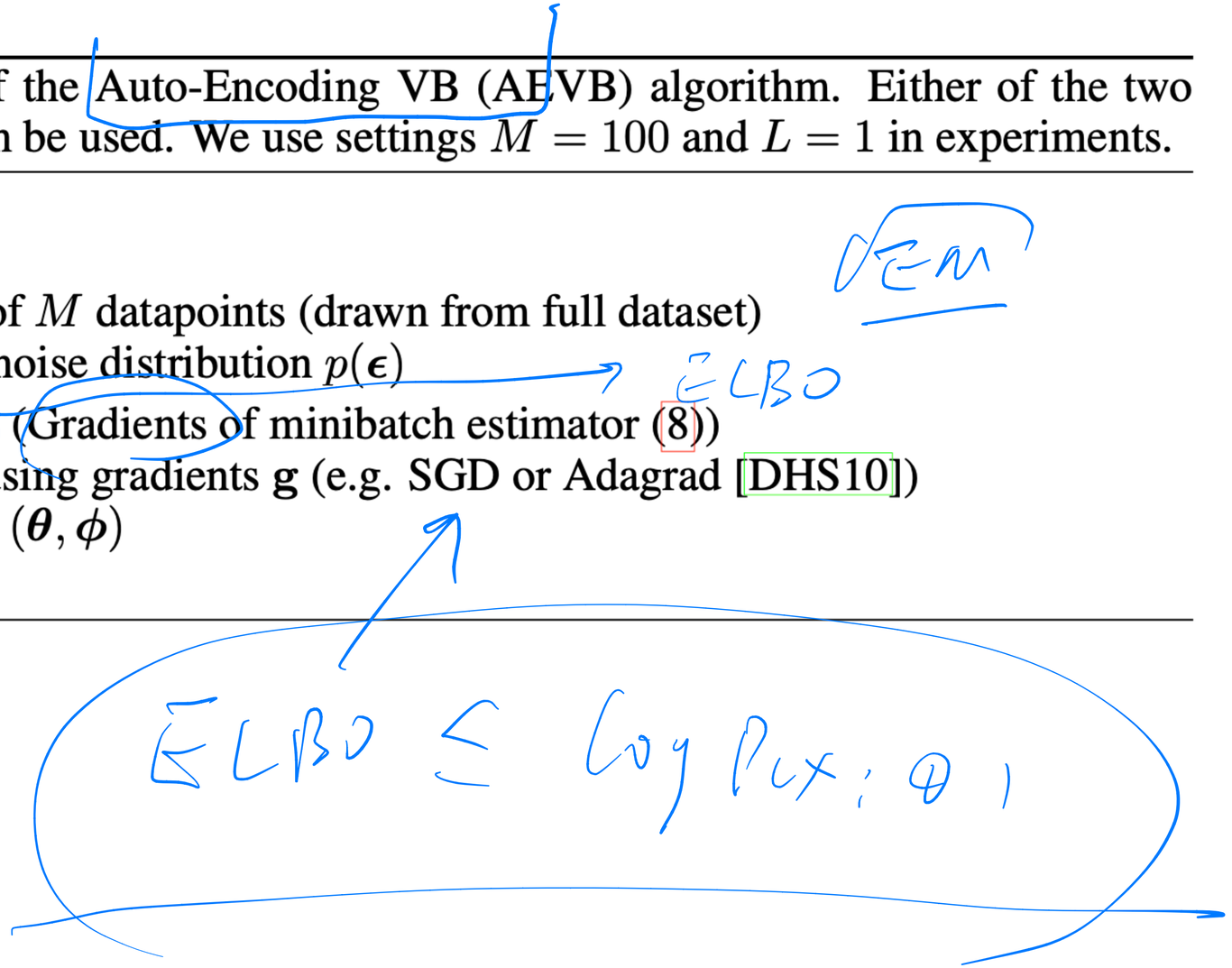

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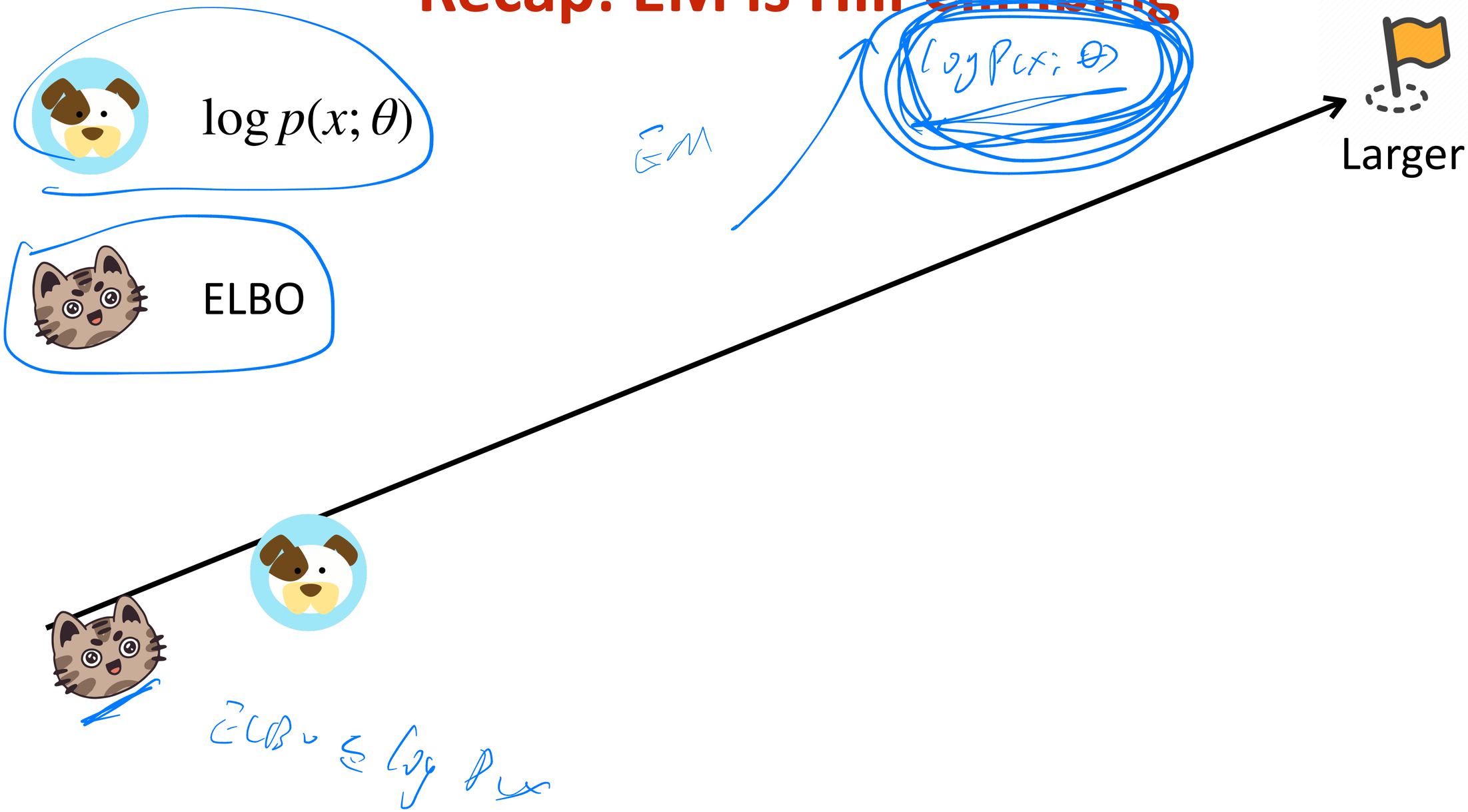
VAE training is optimizing ELBO with gradient descent

Recap: EM is Hill Climbing



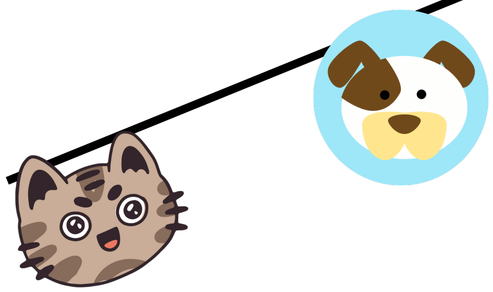
Recap: EM is Hill Climbing

$\log p(x;\theta)$

Only related to θ, no z

ELBO

Larger



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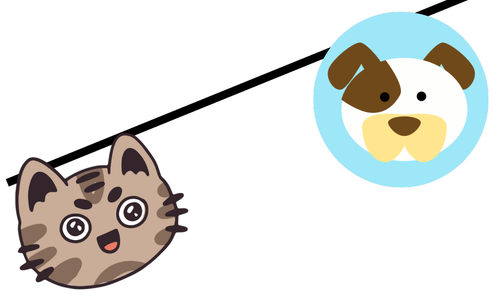
ELBO

Larger



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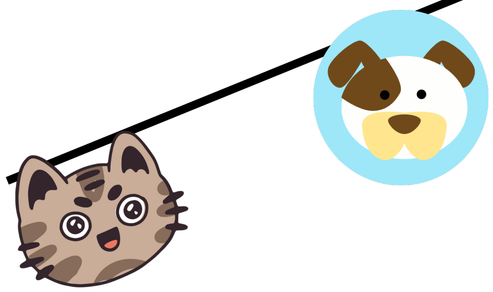


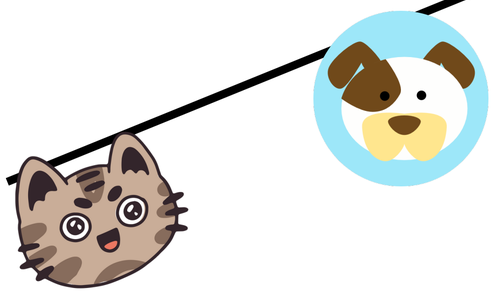
E-step: $Q(z) = p(z \mid x;\theta)$, making ELBO tight

Recap: EM is Hill Climbing

$\log p(x;\theta)$

ELBO

Larger



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"dog" doesn't change, because θ does not change

Recap: EM is Hill Climbing

$\log p(x;\theta)$

ELBO

Larger

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Recap: EM is Hill Climbing

$\log p(x;\theta)$ $\geq$ ELBO

ELBO

Larger

M-step: $\max_{\theta} ELBO$

$\Rightarrow$

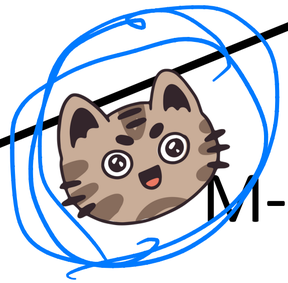
ELBO becomes larger, and it is not tight anymore because posterior changes

Recap: EM is Hill Climbing

$\log p(x;\theta)$

ELBO

Larger



M-step: $\max_{\theta} ELBO$

ELBO becomes larger, and it is not tight anymore because posterior changes

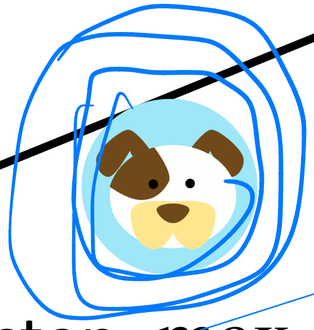
Recap: EM is Hill Climbing

$\log p(x;\theta)$

increase

Larger

ELBO



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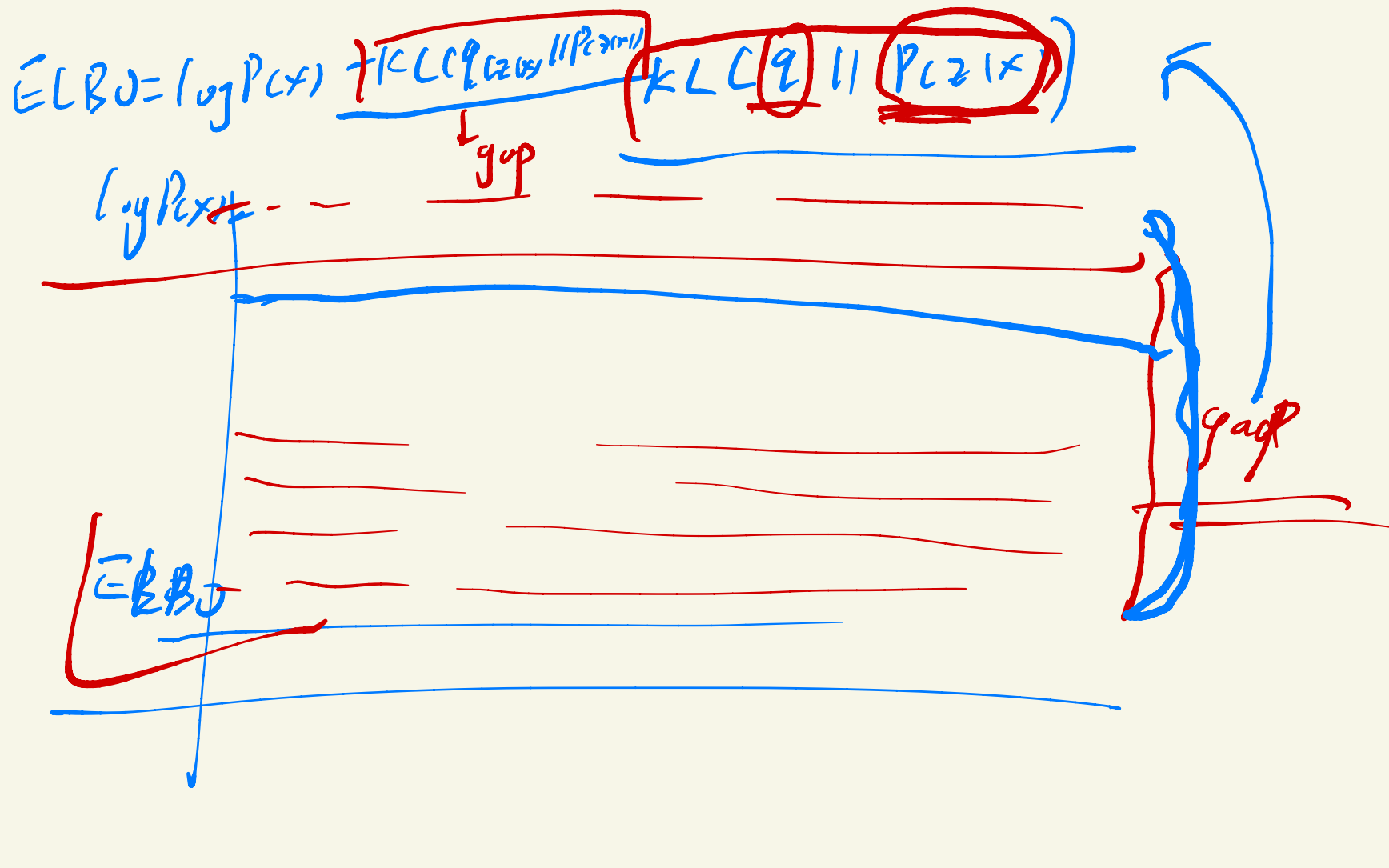
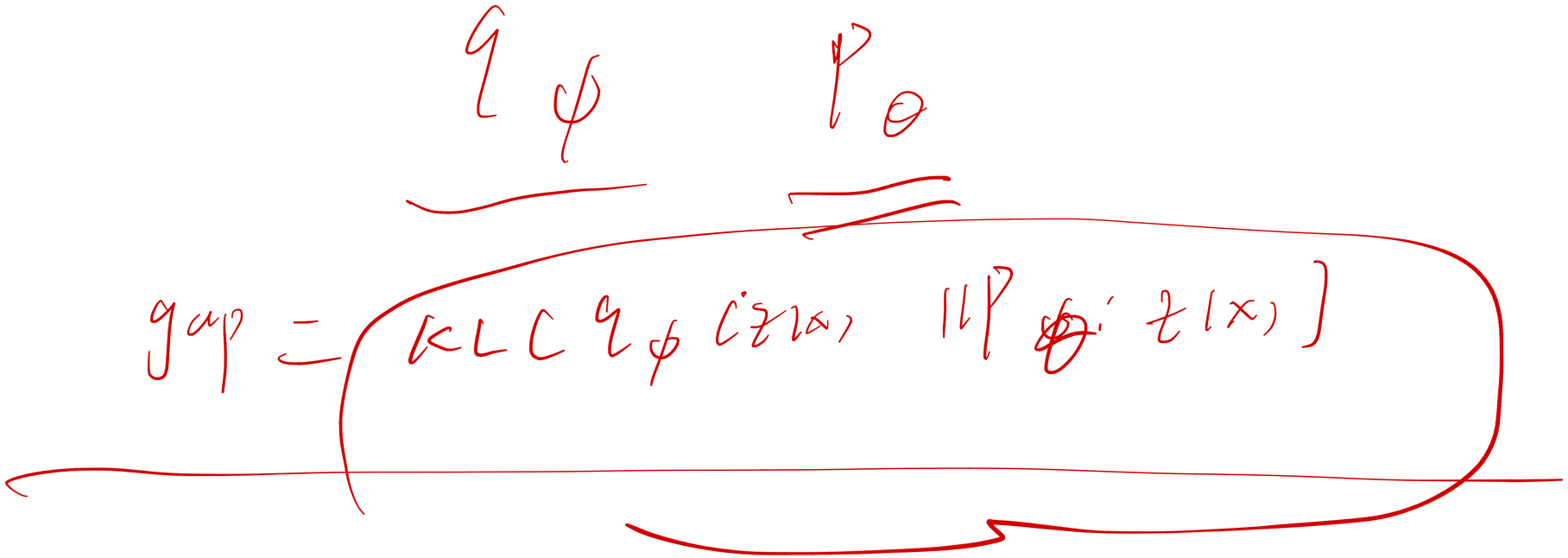

ELBO = log P(x) - KL(q(z|x) || p(z|x)) + KL(q(z|x) || p(z))
gap
log P(x)
ELBO
gap

Is VAE training still Hill Climbing?



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It is not, because $q(z|x)$ may not be accurate to approximate $p(z|x)$

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According to EM, ϕ should be optimized to convergence to have a good approximation for p(z|x) before conducting the M-step, but VAE does not

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It just works in many cases

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The Posterior Collapse Issue

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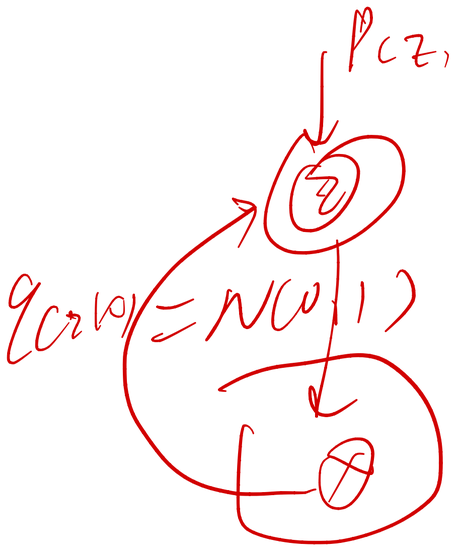
In practice, it is often found that after training, $q_\phi(z \mid x) = p(z)$ and z and x becomes independent (especially in applications of NLP)



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$0 < \lambda < 1$

Reconstruction Loss - λ * KL regularizer

The Posterior Collapse Issue

ELBO

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could be > log P(x)

Reconstruction Loss - λ * KL regularizer

> ELBO

This is not a lower-bound of log p(x) anymore and it breaks MLE, but what is wrong with MLE?

Is VAE training still Hill Climbing?

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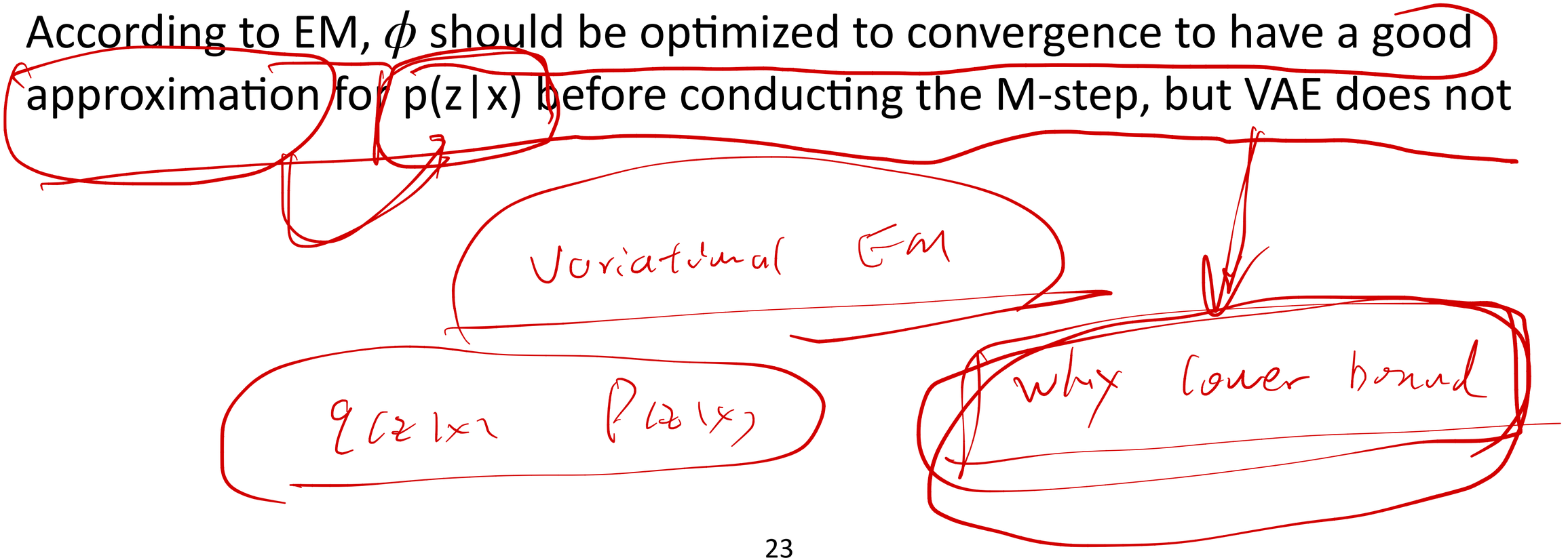

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Can we make it closer to EM to have good guarantees?

VAE training that is Closer to EM

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At every iteration, perform multiple gradient updates of ϕ (E-step) before performing one step of θ (M-step)

VAE training that is Closer to EM

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Published as a conference paper at ICLR 2019

LAGGING INFERENCE NETWORKS AND POSTERIOR COLLAPSE IN VARIATIONAL AUTOENCODERS

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