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

COMP 5212
Machine Learning
Lecture 21

Variational Autoencoders

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Auto-Encoding Variational Bayes

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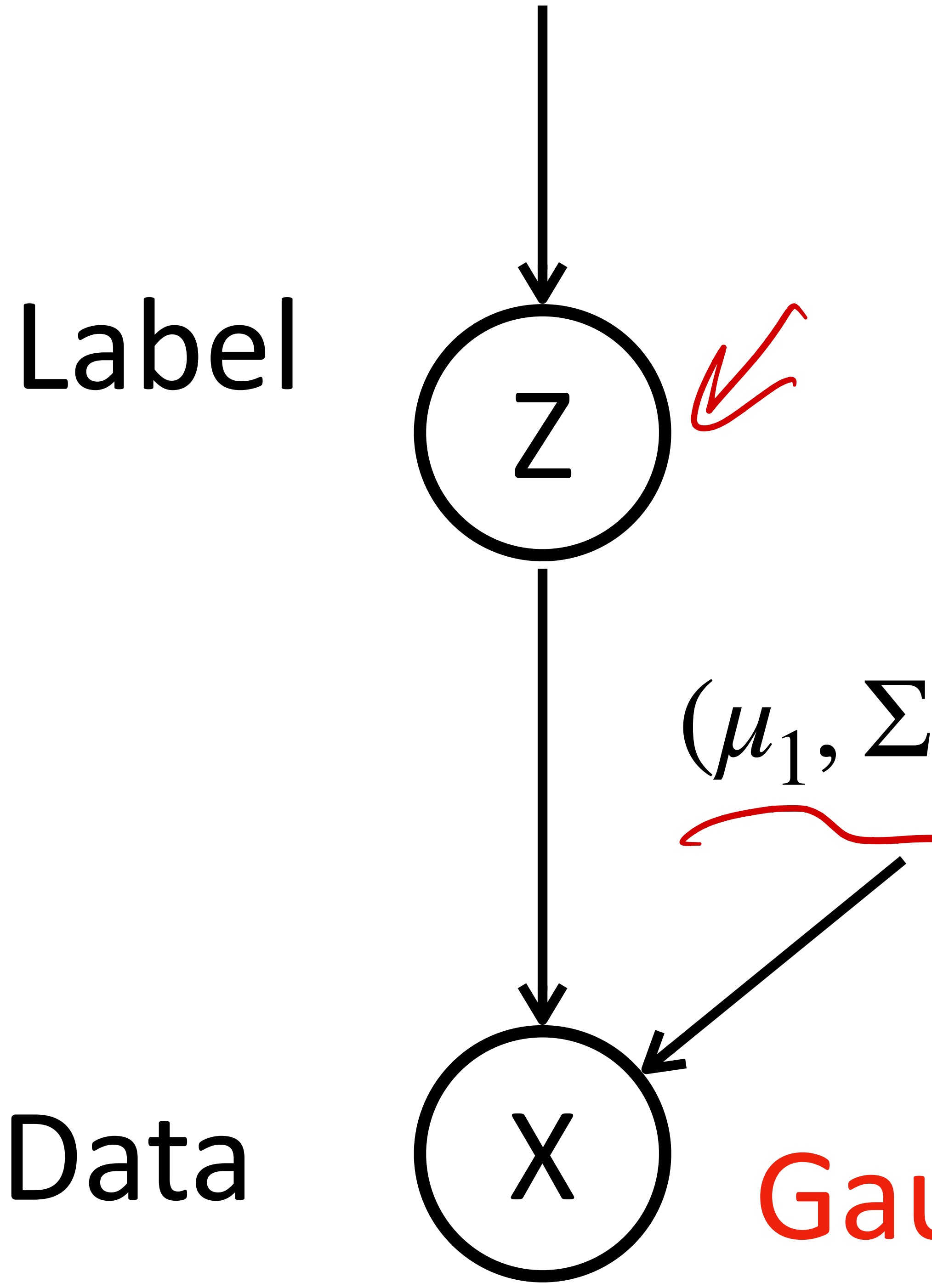
The first test-of-time award in ICLR

VAE is a Generative Model

p(z): multinomial , k classes(e.g. uniform)

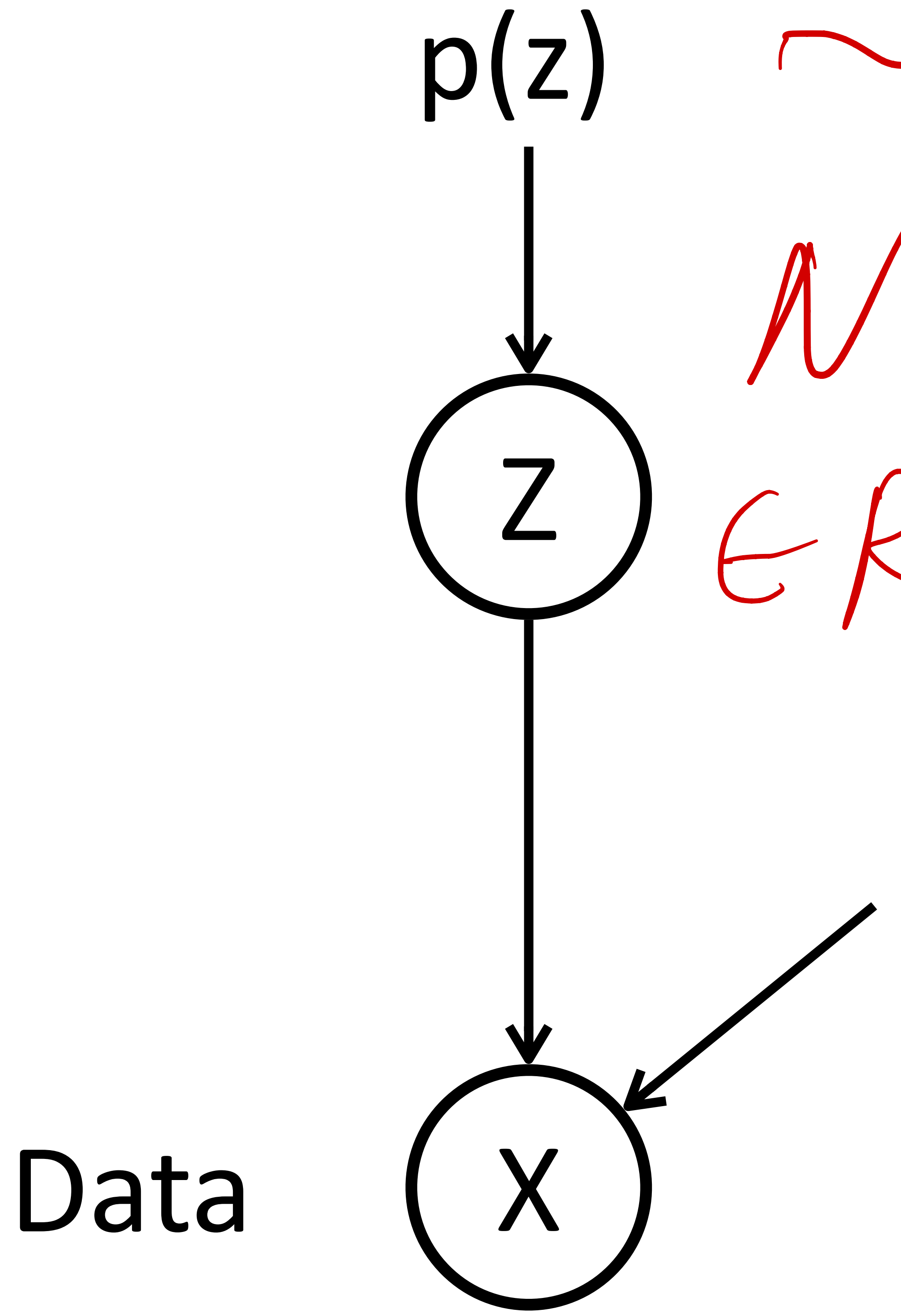


$$(\mu_1, \Sigma_1), (\mu_2, \Sigma_2), \ldots (\mu_k, \Sigma_k)$$

Gaussian Mixture Model (GMM)

The VAE Model

p(z) is a normal distribution in most cases

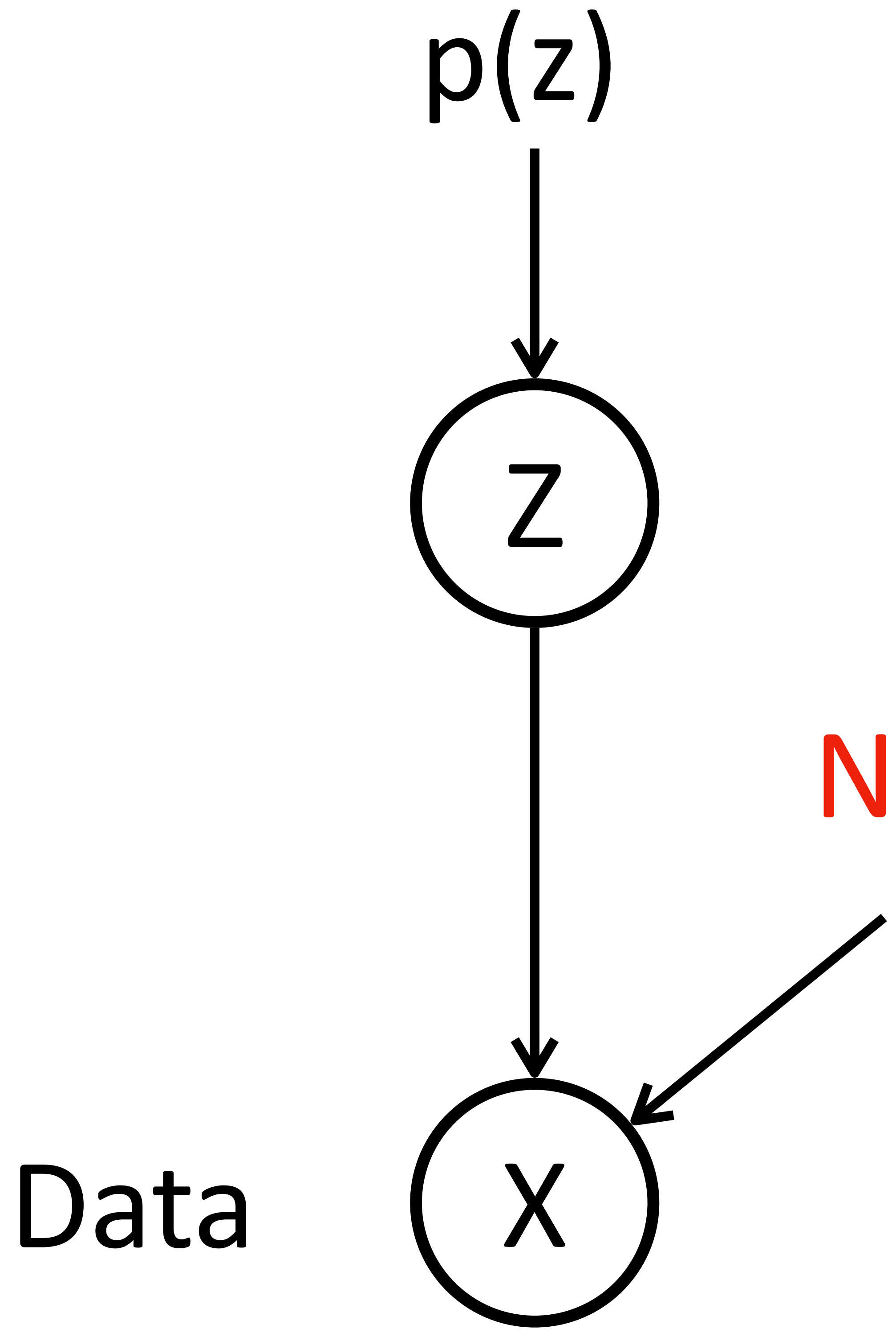


$\mathcal{N}(0, I)$

$\in \mathbb{R}^d$

The VAE Model

p(z) is a normal distribution in most cases

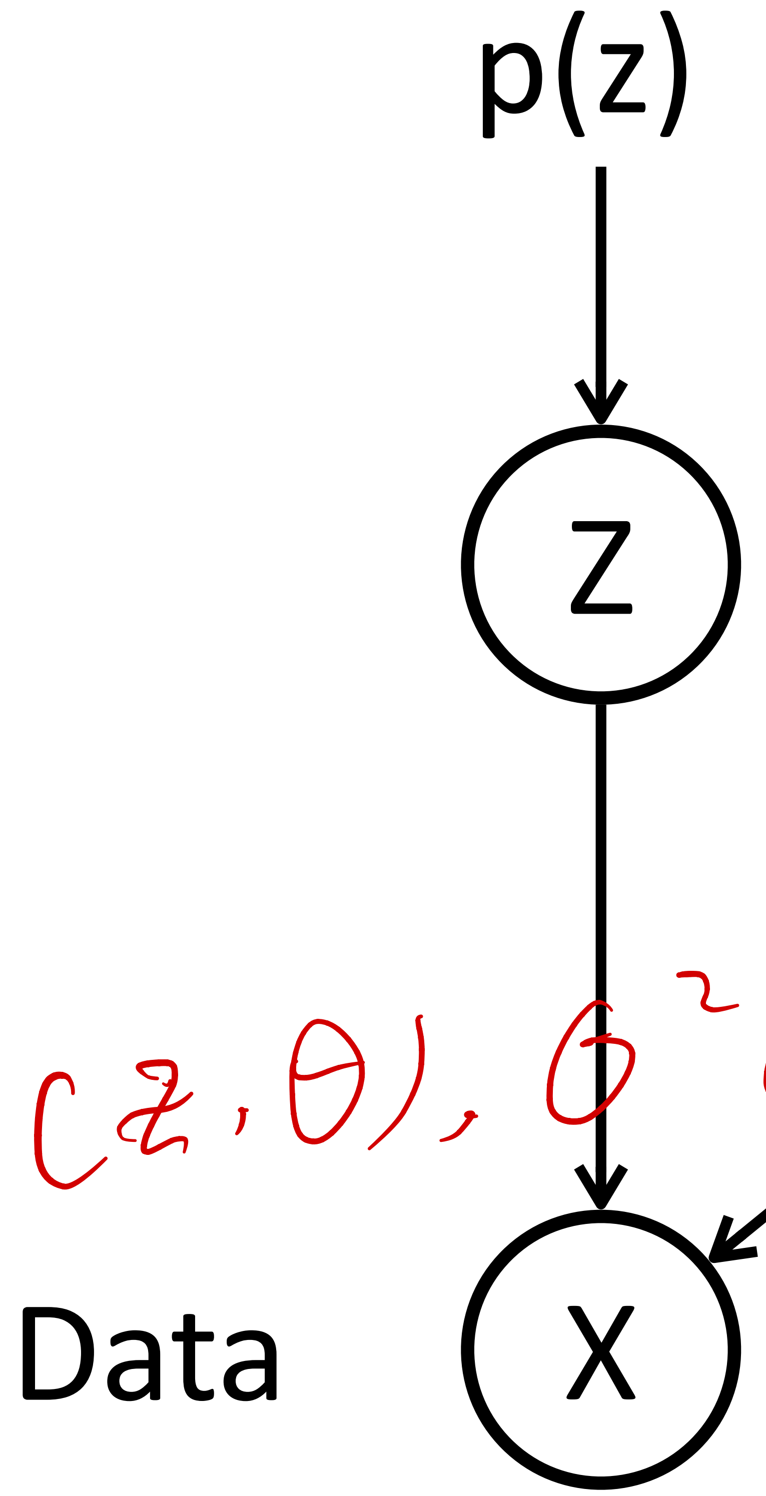


Neural Networks

$P(x|z;$

The VAE Model

p(z) is a normal distribution in most cases



$P(x|z) \sim N(\mu(z,\theta), \sigma^2(z,\theta))$

Neural Networks

$\boxed{NN}$ θ

z parameter

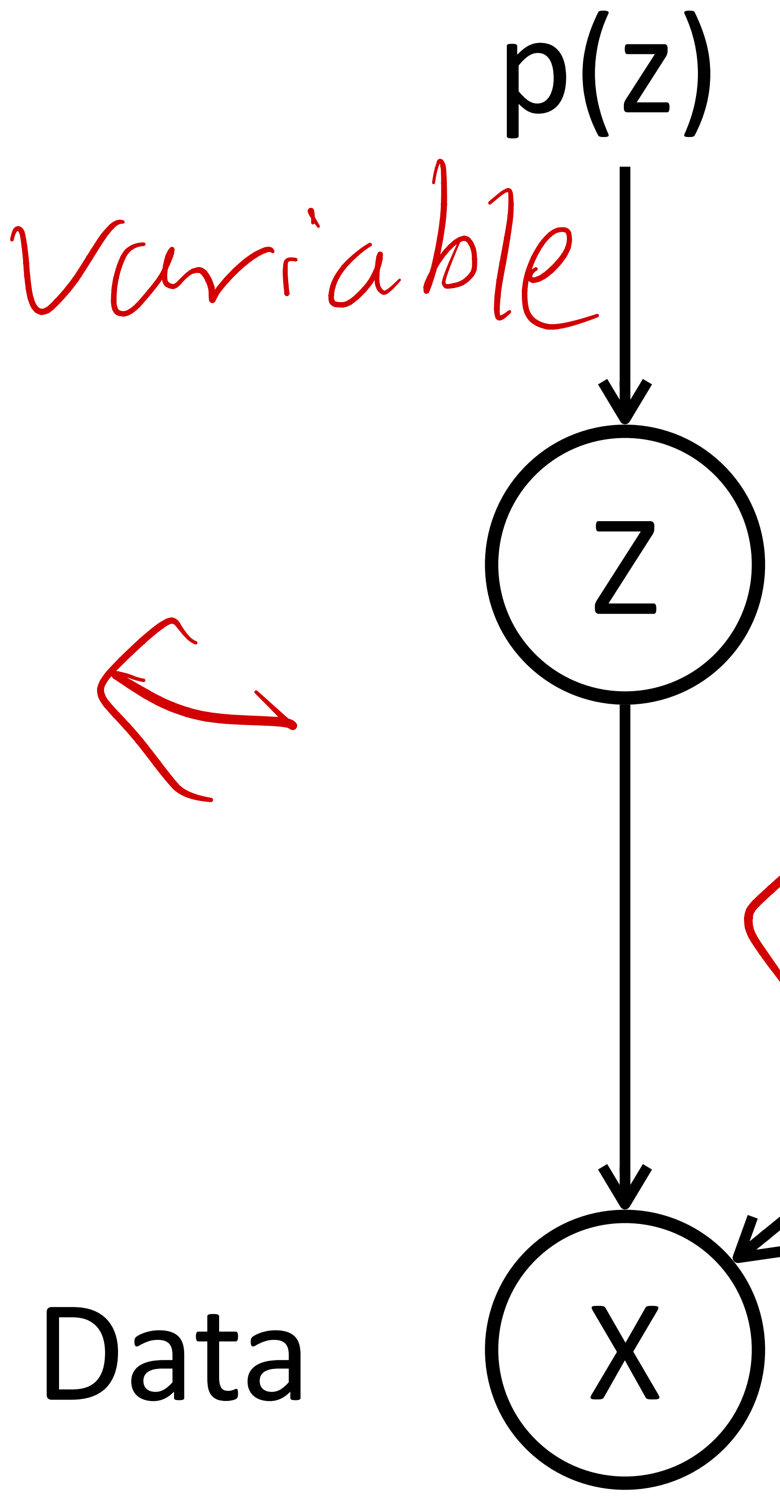
$$X \sim P(x, f(z;\theta))$$

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

The VAE Model

p(z) is a normal distribution in most cases

deep latent-variable model

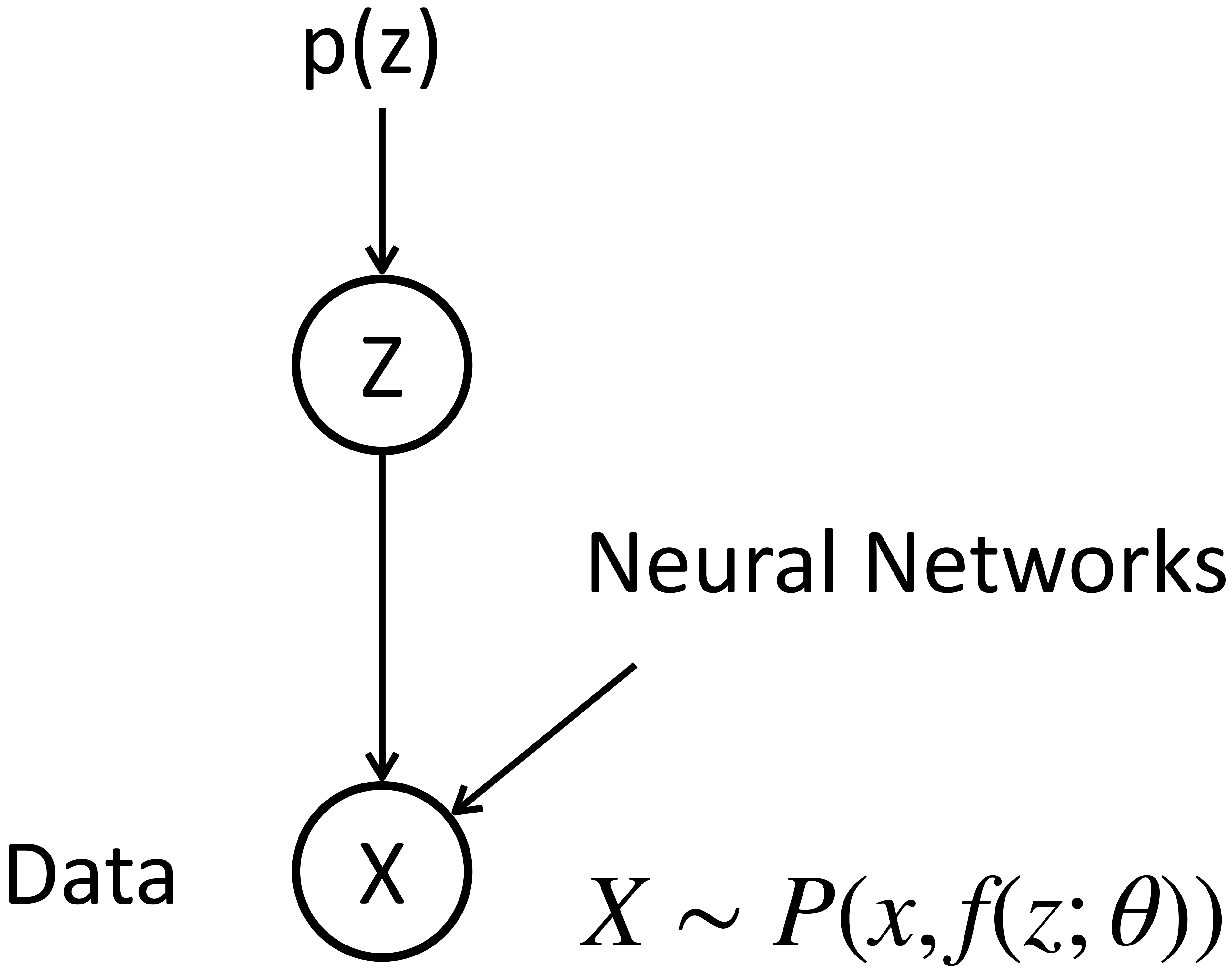


Neural Networks

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

f is a neural network taking Z as input

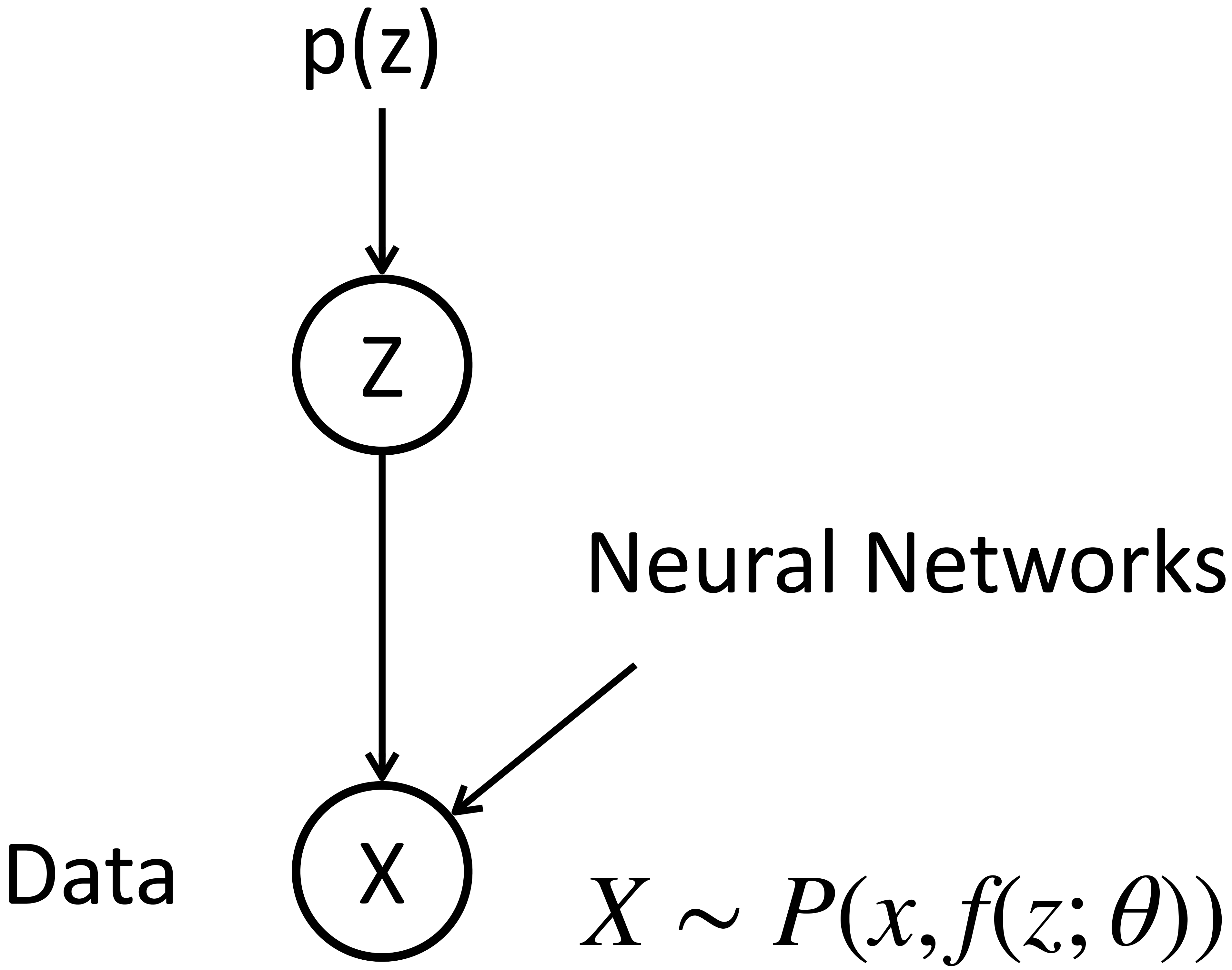
Training



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

$$P(x, z) = \underbrace{P(z)}_{N(0,1)} \underbrace{P(x|z)}_{N(\mu(z;\theta),\ \sigma^2(z;\theta))}$$

Training

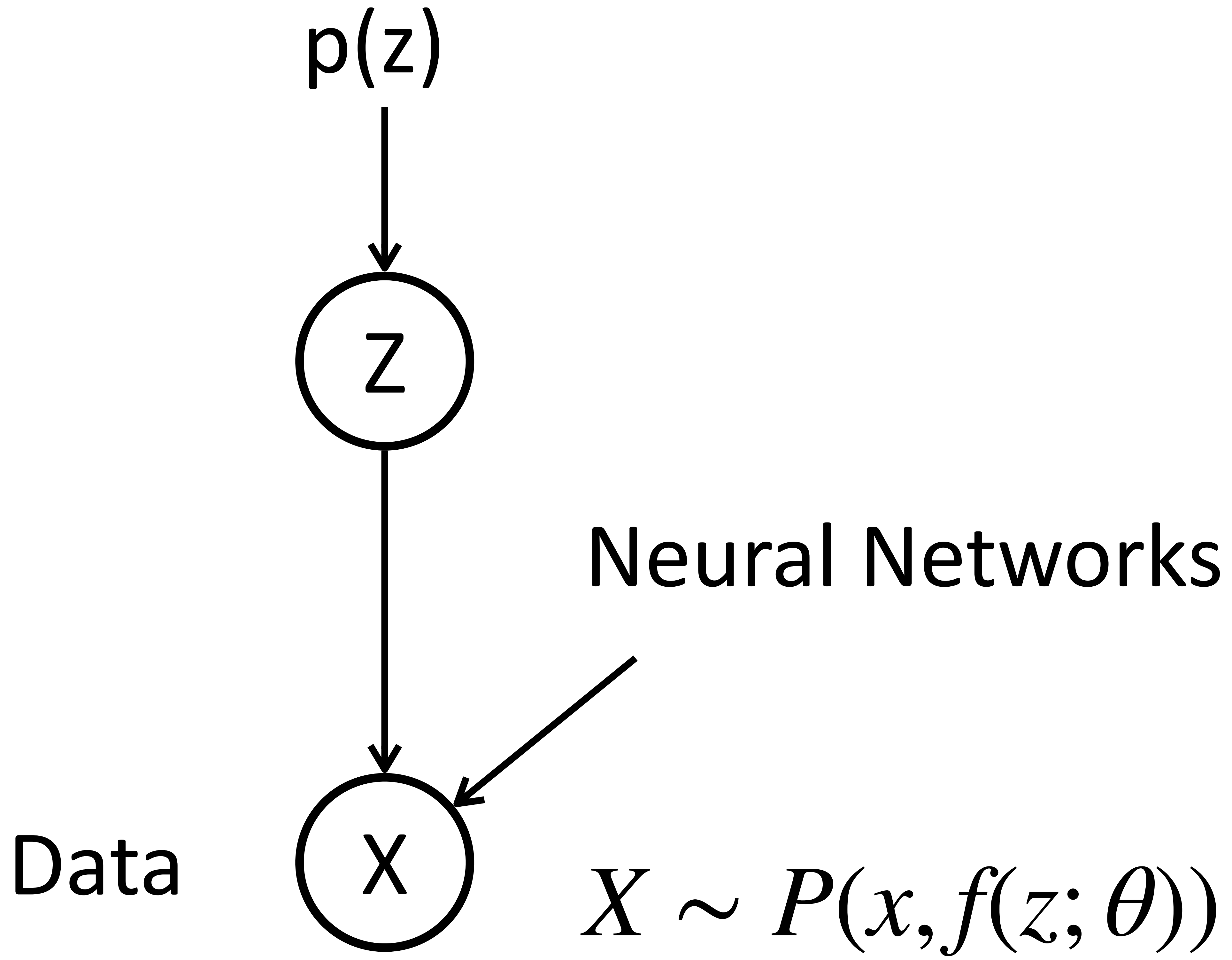


$X \sim P(x, f(z; \theta))$

How to train the model? Can we do MLE?

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

Training

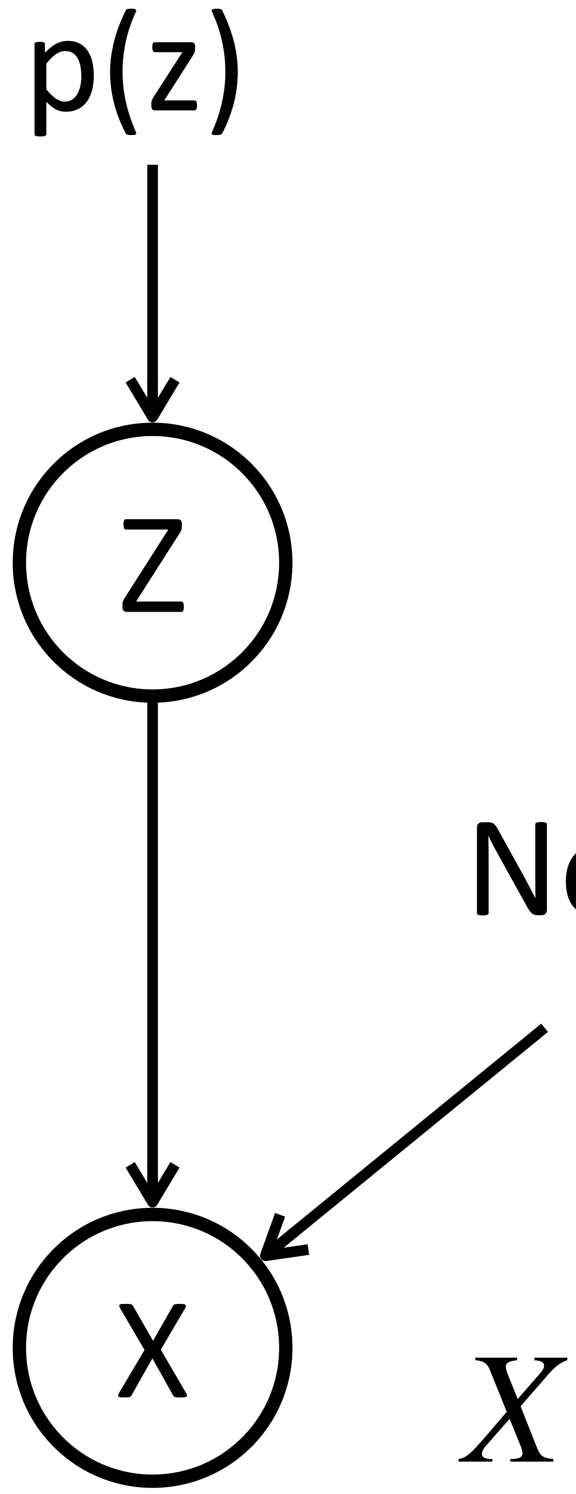


$X \sim P(x, f(z; \theta))$

How to train the model? Can we do MLE?

Intractable P(X), EM algorithm?

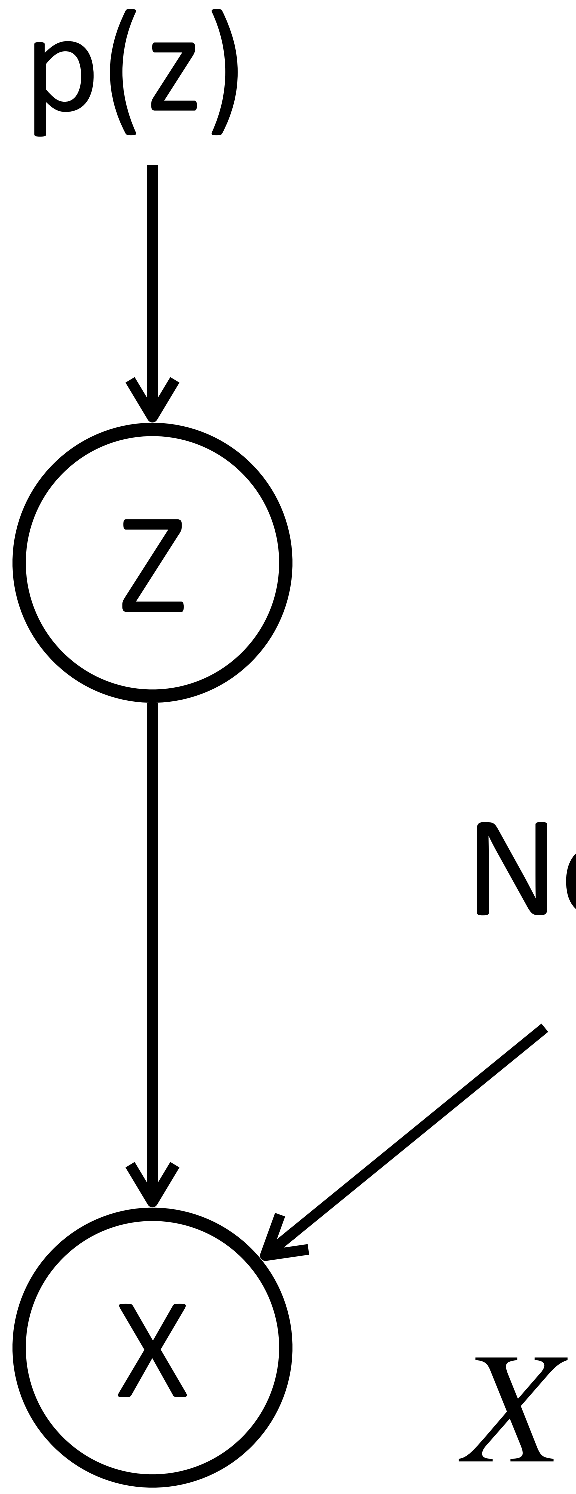
Let's try EM



Neural Networks

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

Let's try EM



Neural Networks

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

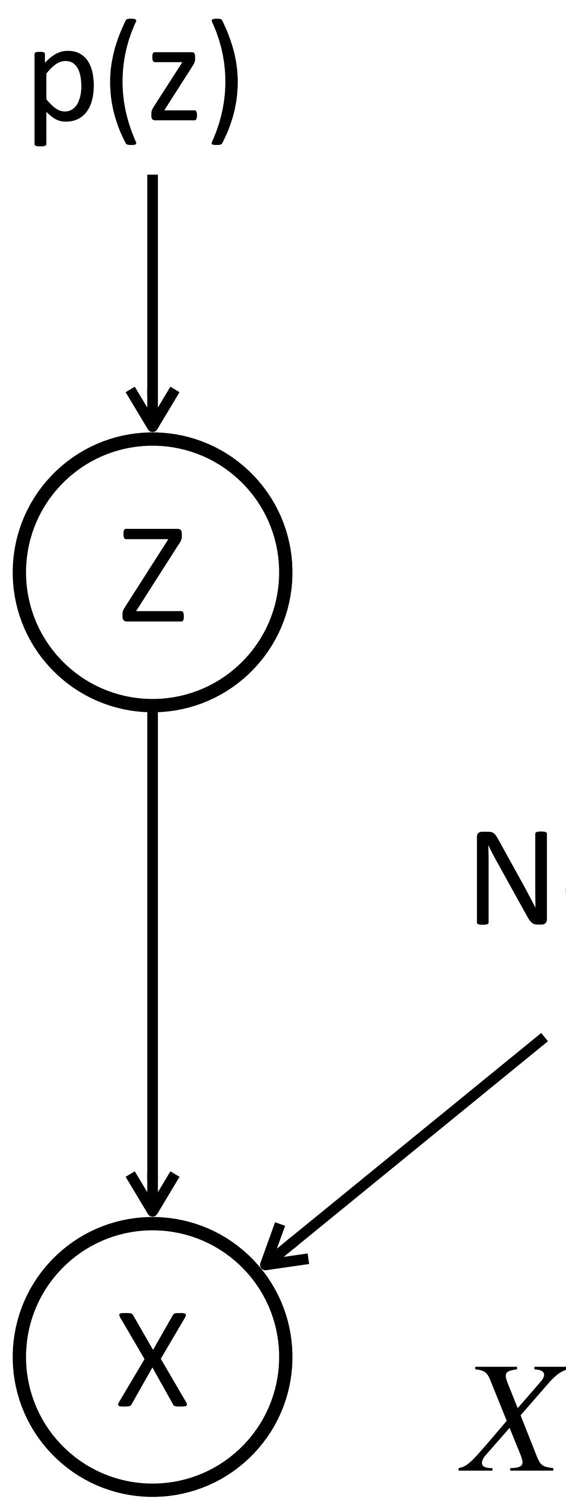
E-Step: compute P(z|x)

$\boxed{P(z|X)}$

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

$P(x, z)$

Let’s try EM



Neural Networks

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

E-Step: compute P(z|x)

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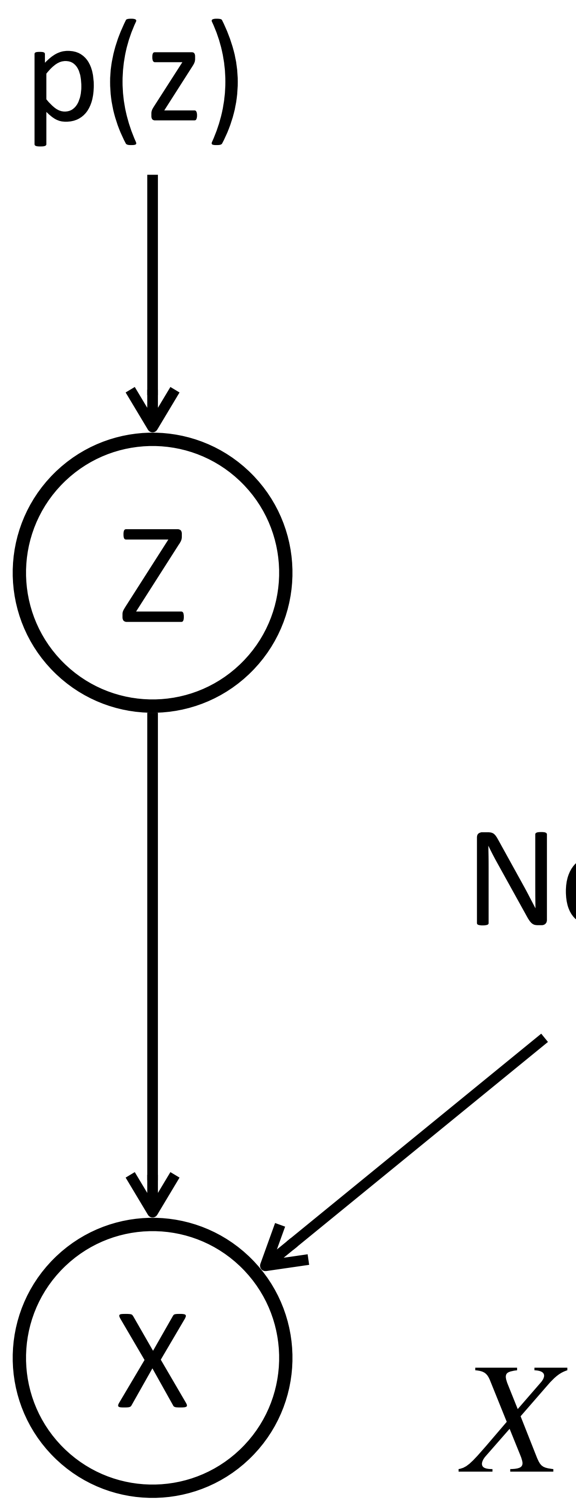
This is ok?

Let's try EM



Neural Networks

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

E-Step: compute P(z|x) → Not Gaussian

$$Q(z) = P(z\,|\,x) \propto P(z)P(x\,|\,z)$$

This is ok?

$P(z) \sim N(0, 1)$

$P(x|z) \sim N(\mu(z), \sigma(z)^2)$

M-Step: the ELBO objective

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

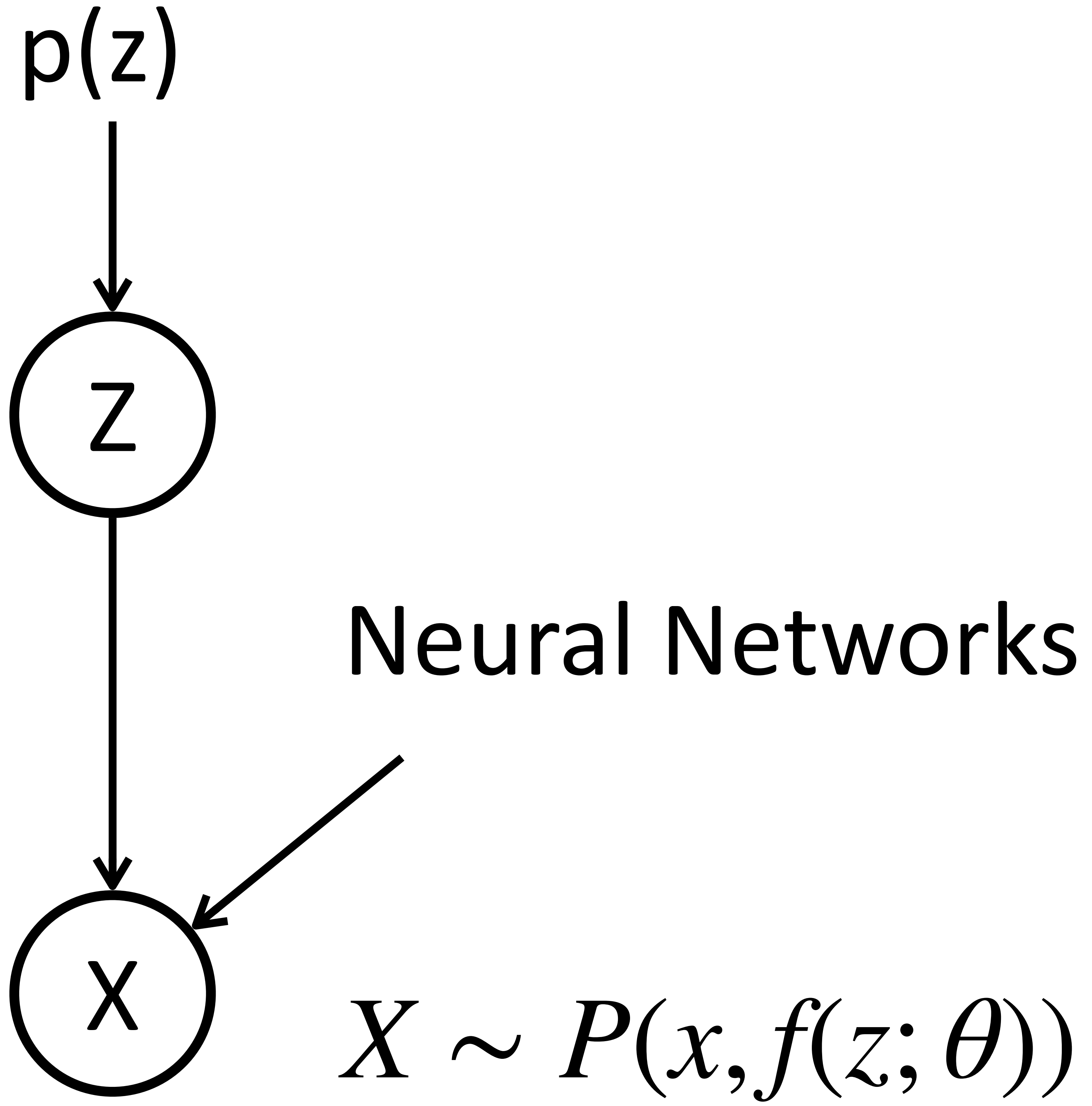
x $P(x) = ?$

$x \sim P(x)$

$(z \sim Q(z))$

Monte Carlo samples

Let's try EM



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

$\mathcal{N}(0,1)$

E-Step: compute P(z|x)

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

This is ok? $P(x|z)$

$P(z|x) = f(z)$

NN

z

x

M-Step: the ELBO objective

cannot

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

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

$$p(z|x)$$

$$p(x|z) \sim N(\mu(z;\theta), \sigma^2(z;\theta))$$

$$= \frac{1}{\sqrt{2\pi}|\Sigma|} \exp((x-\mu)^T \Sigma^{-1} (x-\mu))$$

$$p(x|z) =$$

$$\mu = NN(z)$$

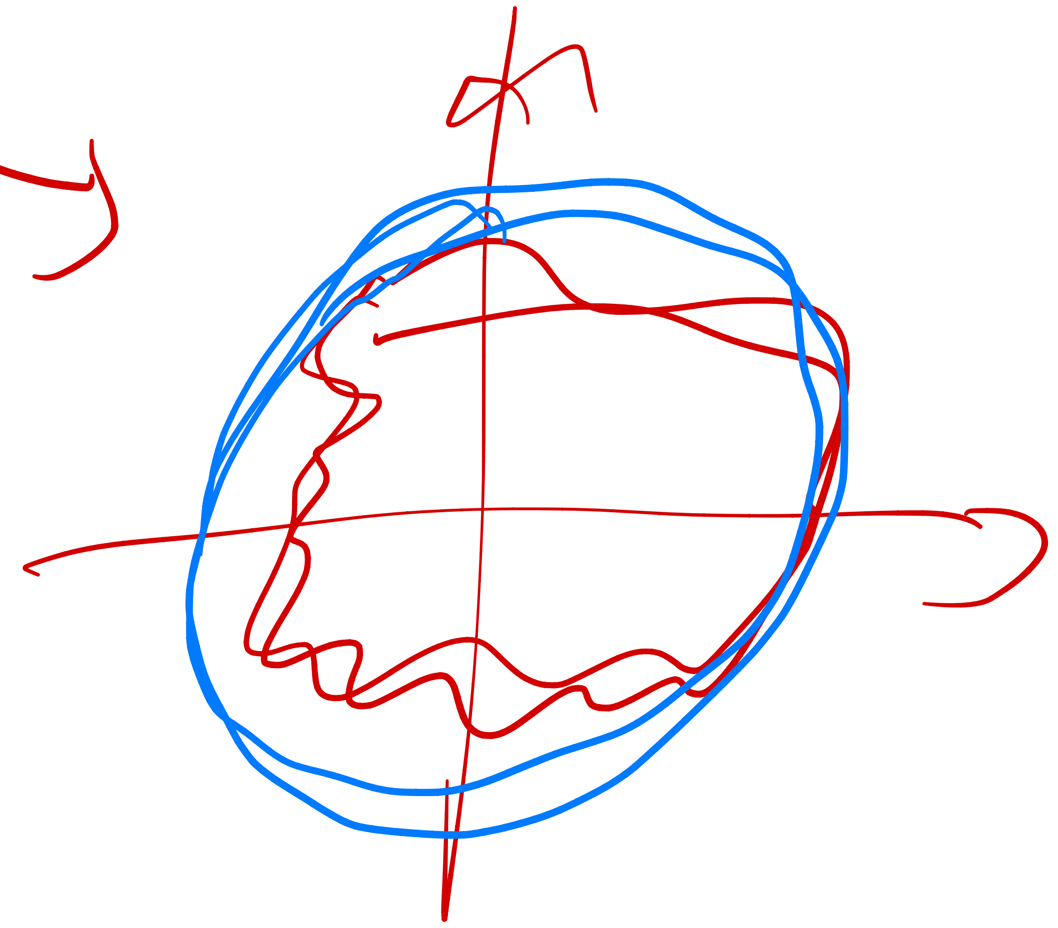
Approximate Posterior

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

Approximate Posterior

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

$q(z \mid x; \phi)$ to approximate $p(z \mid x; \theta)$



Approximate Posterior

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ϕ is the parameter for the approximate function, θ is the generative model parameter

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

Approximate Posterior

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

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

ϕ is the parameter for the approximate function, θ is the generative model parameter

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

?

It needs to be some distance metric between $q(z \mid x; \phi)$ and $p(z \mid x; \theta)$

$KL(q \| p(z|x))$

$KL(q \,\|\, p) =$

$$ELBO = \log p_\theta(x) - \underbrace{KL(q \,\|\, p(z|x))}$$

EL

Recap: ELBO

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

Jensen inequality

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

$Q \leftarrow q(z|x;\phi)$

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

$\Downarrow$

$\text{ELBO} = \log P(x)$

$Q(z) \neq P(z|x)$

$\Downarrow$

$\text{ELBO} < \log P(x)$

Recap: ELBO

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

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

fixed

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

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

θ is fixed

Recap: ELBO

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

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

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

Maximizing ELBO is equivalent to minimize the KL divergence

$$\mathrm{ELBO}(x; Q, \theta) = \log p(x) - D_{KL}(Q \| p_{z|x})$$

fixed

$Q \longrightarrow P(z|x)$

$$\boxed{ELBO = E_{x \sim Q(z)}\left[\log P(x|z)\right] - KL(Q(z)\|P(z))}$$

$P(z)$

$$\boxed{ELBO = \log P(x) - KL(Q(z)\|P(z|x))}$$

$$= \log P(x) - \int_z Q(z) \log \frac{Q(z)}{P(z|x)}$$

$$\frac{P(x,z)}{P(x)}$$

$$= \log P(x) - \int_z Q(z) \log \frac{Q(z)P(x)}{P(x,z)}$$

$$\mathrm{ELBO} = \log P(x) - \int_z Q(z) \log \frac{Q(z)\, P(x)}{P(x, z)}$$

$$= \log P(x) - \int_z Q(z) \left[\log Q(z) + \log P(x) - \log P(x, z) \right]$$

$$= \cancel{\log P(x)} - \int_z Q(z) \log Q(z) - \boxed{\underbrace{\int_z Q(z)}_{1} \log P(x)} + \int_z Q(z) \log P(x, z)$$

$$\cancel{\log P(x)}$$

$$= -\int_z Q(z) \log Q(z) + \int_z Q(z) \left[\log P(x \mid z) + \underline{\log P(z)} \right]$$

$$= E_{z \sim Q(z)} \log P(x \mid z) - KL\left(Q(z) \,\|\, P(z) \right) \in$$

Recap: ELBO

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

Maximizing ELBO is equivalent to minimize the KL divergence

$$\mathrm{ELBO}(x; Q, \theta) = \log p(x) - D_{KL}(Q \| p_{z|x})$$

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

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

Gaussian

$q(z|x;\phi) \xrightarrow{\text{closer}} p(z|x)$

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

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

Recap: ELBO

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

Maximizing ELBO is equivalent to minimize the KL divergence

$$\mathrm{ELBO}(x; Q, \theta) = \log p(x) - D_{KL}(Q \| p_{z|x})$$

P(S|D)

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

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

exact inference

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

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

Variational Inference

Training VAEs

E-Step:

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

ELBO

M-Step:

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

ELBO

Training VAEs

E-Step:

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

M-Step:

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

Same objective, different parameters to optimize

Training VAEs

E-Step:

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

M-Step:

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

ϕ

θ

Same objective, different parameters to optimize

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

Training VAEs

E-Step:

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

M-Step:

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

Training VAEs

sigmoid

linear $(x;\phi)$

E-Step:

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

$q(z|x;\phi) = N(\mu(x;\phi), \sigma^2(x;\phi))$

M-Step:

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

NN

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

Training VAEs

E-Step:

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

Can we do gradient descent over ϕ?

$E_{z\sim q(z|x;\phi)}[\log[\cdots]]$

M-Step:

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

$z_0 \sim q(z|x;\phi)$

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

A Common Choice for $q(z \mid x; \phi)$

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$$q(z \mid x; \phi) = N(\mu, \sigma^2)$$

$$\mu, \sigma = g(x; \phi)$$

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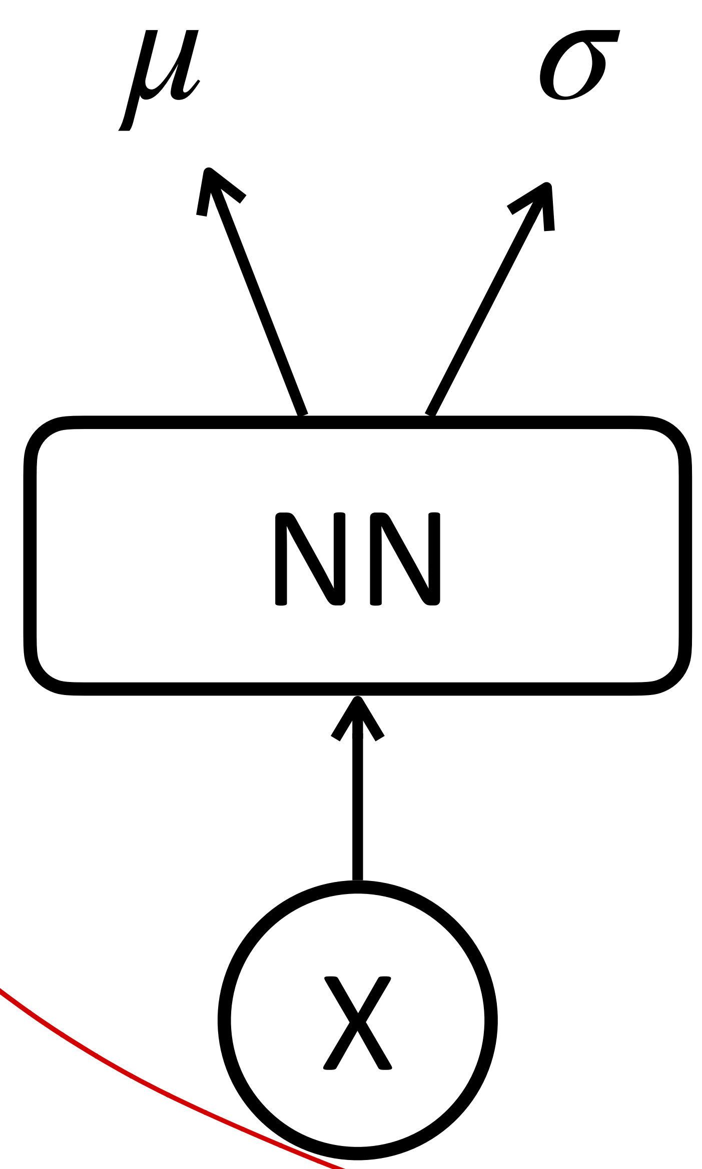

Inference model/network

Training VAEs

E-Step:

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

M-Step:

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

Training VAEs

E-Step:

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Same objective, different parameters to optimize

Training VAEs

E-Step:

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

Training VAEs

E-Step:

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We use MC sampling to approximate expectation
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Training VAEs

E-Step:

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

Can we do gradient descent over ϕ?

M-Step:

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

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

Reparameterization Trick

E-Step:

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

Reparameterization Trick

E-Step:

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

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

Reparameterization Trick

E-Step:

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

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?

Try to express z as a deterministic function $z = g_{\phi}(\epsilon, x)$, where ϵ is an auxiliary random variable

$z_0 \sim N(\mu, \sigma)$

$z_0 = g(\mu, \sigma)$

Reparameterization Trick

E-Step:

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

gradient descent

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

Try to express z as a deterministic function $z = g_\phi(\epsilon, x)$, where ϵ is an auxiliary random variable

$z \sim N(\mu, \sigma^2)$

$$z \sim N(\mu, \sigma^2) \longrightarrow \boxed{z = \mu + \sigma \odot \epsilon,} \quad \epsilon \sim N(0,1)$$

Reparameterization Trick

E-Step:

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Try to express z as a deterministic function $z = g_\phi(\epsilon, x)$, where ϵ is an auxiliary random variable

$\mathcal{N}(\mu, \sigma^2)$

$$z \sim N(\mu, \sigma^2) \longrightarrow z = \mu + \sigma \odot \epsilon, \quad \epsilon \sim N(0,1)$$

Can you verify z in this equation is Gaussian?

Reparameterization Trick

E-Step:

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

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

Reparameterization Trick

E-Step:

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

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

1. Randomly sample $\epsilon^{(i)} \sim N(0,1)$

Reparameterization Trick

E-Step:

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

1. Randomly sample $\epsilon^{(i)} \sim N(0,1)$
2. Obtain z sample as $z^{(i)} = \mu + \sigma \odot \epsilon^{(i)}$

Reparameterization Trick

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1. Randomly sample $\epsilon^{(i)} \sim N(0,1)$
2. Obtain z sample as $z^{(i)} = \mu + \sigma \odot \epsilon^{(i)}$
3. Perform gradient descent w.r.t. $\log \frac{p(x, z^{(i)}; \theta)}{q(z^{(i)} \mid x; \phi)}$

Reparameterization Trick

E-Step:

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1. Randomly sample $\epsilon^{(i)} \sim N(0,1)$
2. Obtain z sample as $z^{(i)} = \mu + \sigma \odot \epsilon^{(i)}$
3. Perform gradient descent w.r.t. $\log\dfrac{p(x,z^{(i)};\theta)}{q(z^{(i)}\,|\,x;\phi)}$

We can now propagate gradients from z to ϕ

Reparameterization Trick

VAE is a class of models

What kind of $q(z \mid x; \phi)$ allows for such a reparameterization trick?

Kingma et al. Auto-Encoding Variational Bayes

Reparameterization Trick

VAE is a class of models

What kind of $q(z \mid x; \phi)$ allows for such a reparameterization trick?

1. Tractable inverse CDF. In this case, let $\epsilon \sim \mathcal{U}(\mathbf{0}, \mathbf{I})$, and let $g_\phi(\epsilon, \mathbf{x})$ be the inverse CDF of $q_\phi(\mathbf{z}|\mathbf{x})$. Examples: Exponential, Cauchy, Logistic, Rayleigh, Pareto, Weibull, Reciprocal, Gompertz, Gumbel and Erlang distributions.
2. Analogous to the Gaussian example, for any "location-scale" family of distributions we can choose the standard distribution (with location $= 0$, scale $= 1$) as the auxiliary variable ϵ, and let $g(.) = \text{location} + \text{scale} \cdot \epsilon$. Examples: Laplace, Elliptical, Student's t, Logistic, Uniform, Triangular and Gaussian distributions.
3. Composition: It is often possible to express random variables as different transformations of auxiliary variables. Examples: Log-Normal (exponentiation of normally distributed variable), Gamma (a sum over exponentially distributed variables), Dirichlet (weighted sum of Gamma variates), Beta, Chi-Squared, and F distributions.

$q(z|x;\phi)$

Kingma et al. Auto-Encoding Variational Bayes

ELBO

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

ELBO

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

ELBO is implemented with the following form:

max

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

$\rightarrow N(0,1)$

z

x

$x \xrightarrow{q} z \xrightarrow{p(x|z)} x$

$p(x|z) \sim N(\mu, \sigma^2)$

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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Autoencoder

AE

x z $\hat{x}$

ELBO

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Autoencoder Loss

ELBO

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

Autoencoder Loss

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

ELBO

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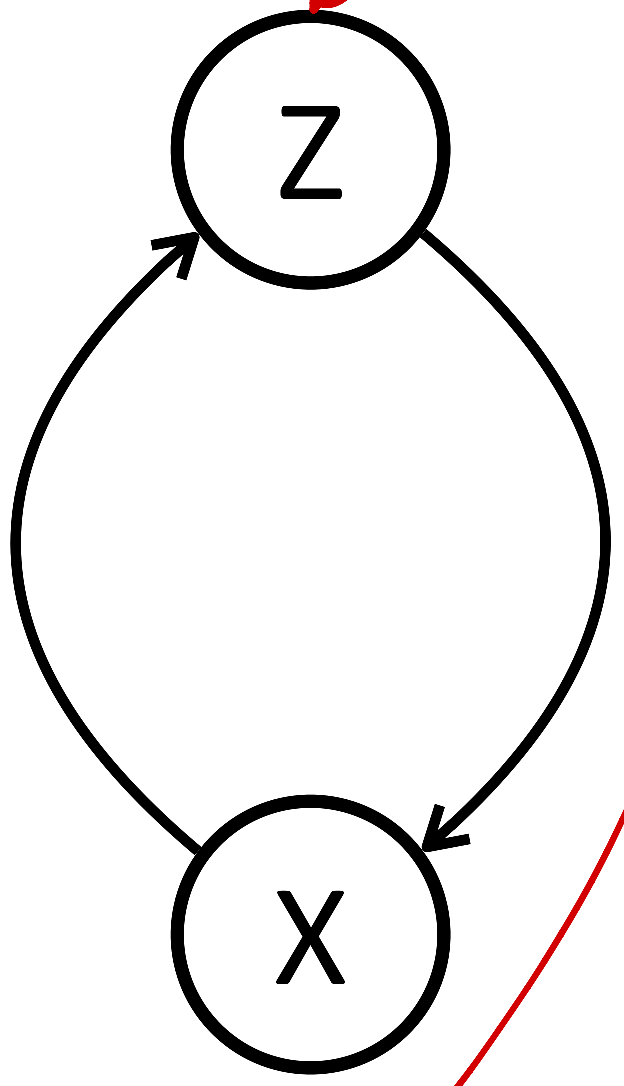
Autoencoder Loss

$p(z)$

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



$p(x)$

$p(z, x)$

ELBO

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

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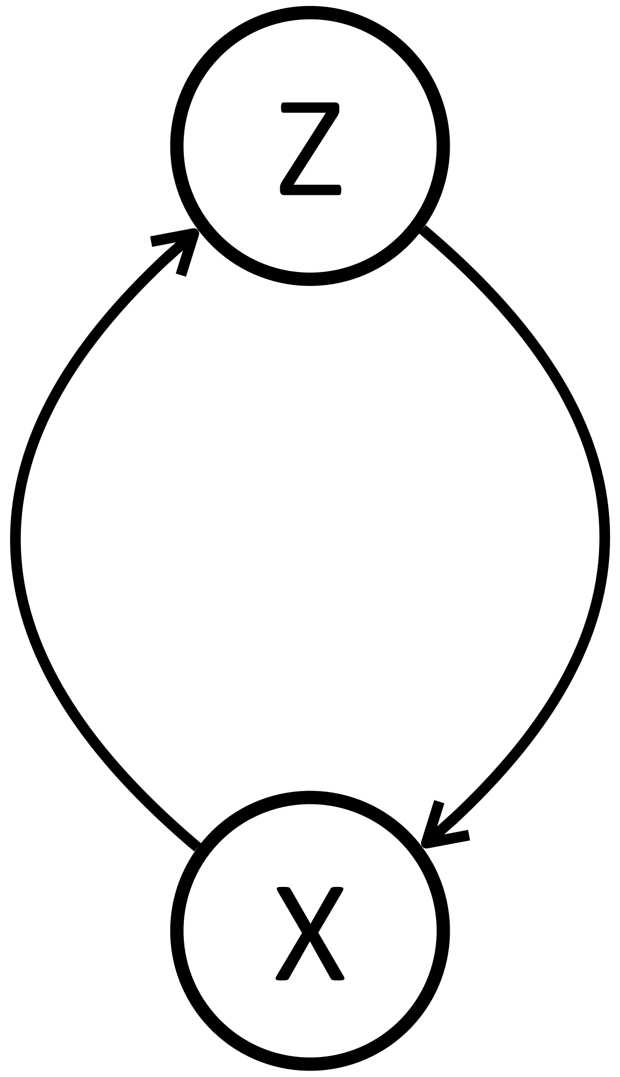

This is why it is called variational "autoencoder"

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

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ELBO

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$$D_{KL}(\mathcal{N}(\mu_1, \sigma_1^2) \| \mathcal{N}(\mu_2, \sigma_2^2))$$

$$-D_{KL}((q_{\boldsymbol{\phi}}(\mathbf{z})\|p_{\boldsymbol{\theta}}(\mathbf{z})) = \int q_{\boldsymbol{\theta}}(\mathbf{z}) \left(\log p_{\boldsymbol{\theta}}(\mathbf{z}) - \log q_{\boldsymbol{\theta}}(\mathbf{z})\right)\, d\mathbf{z}$$
$$\boxed{= \frac{1}{2}\sum_{j=1}^{J}\left(1 + \log((\sigma_j)^2) - (\mu_j)^2 - (\sigma_j)^2\right)}$$

Training VAEs

E-Step:

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

M-Step:

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Training VAEs

$\log P(x) \uparrow$

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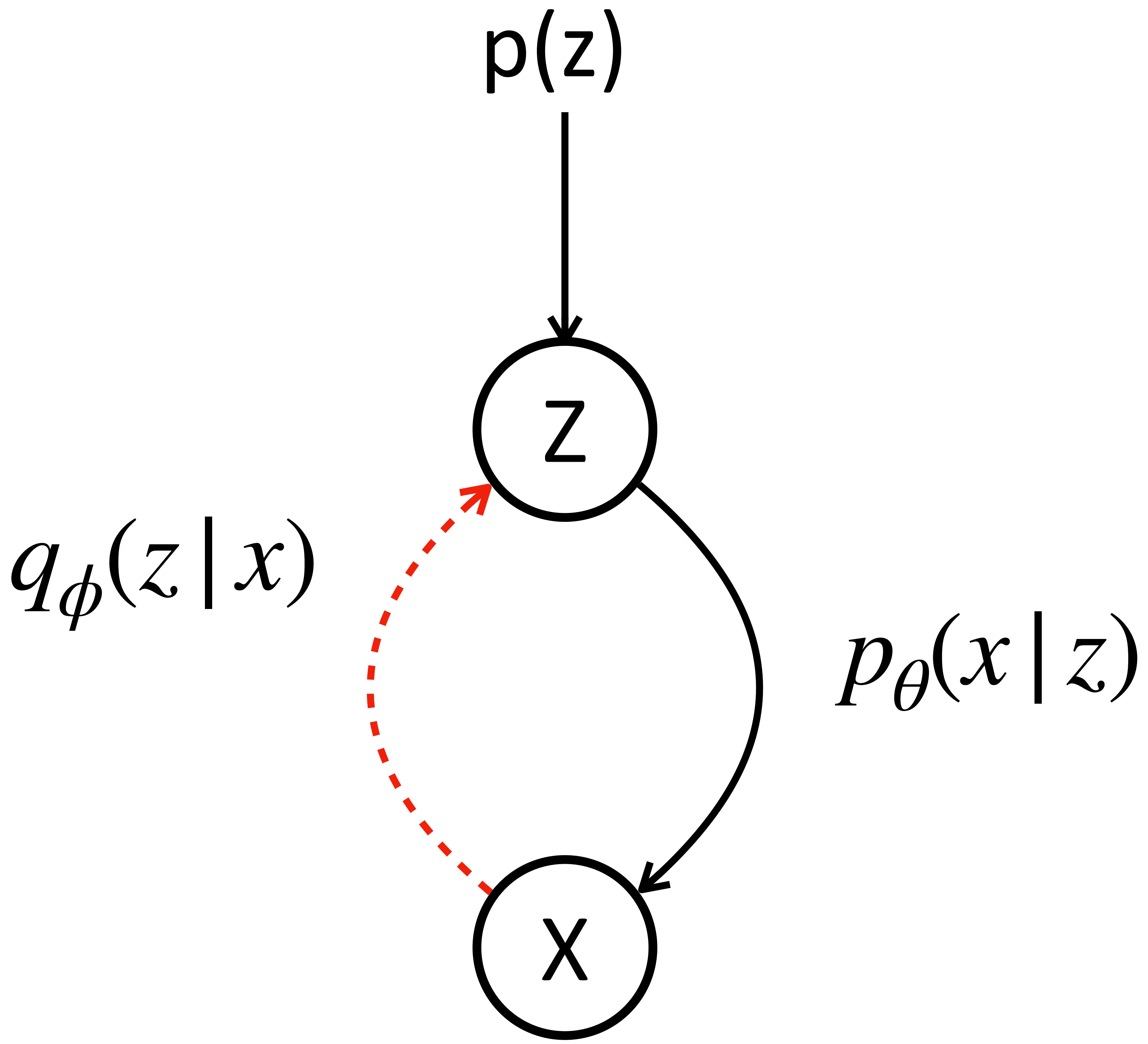
$q(z|x)$

$P(z|x)$

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



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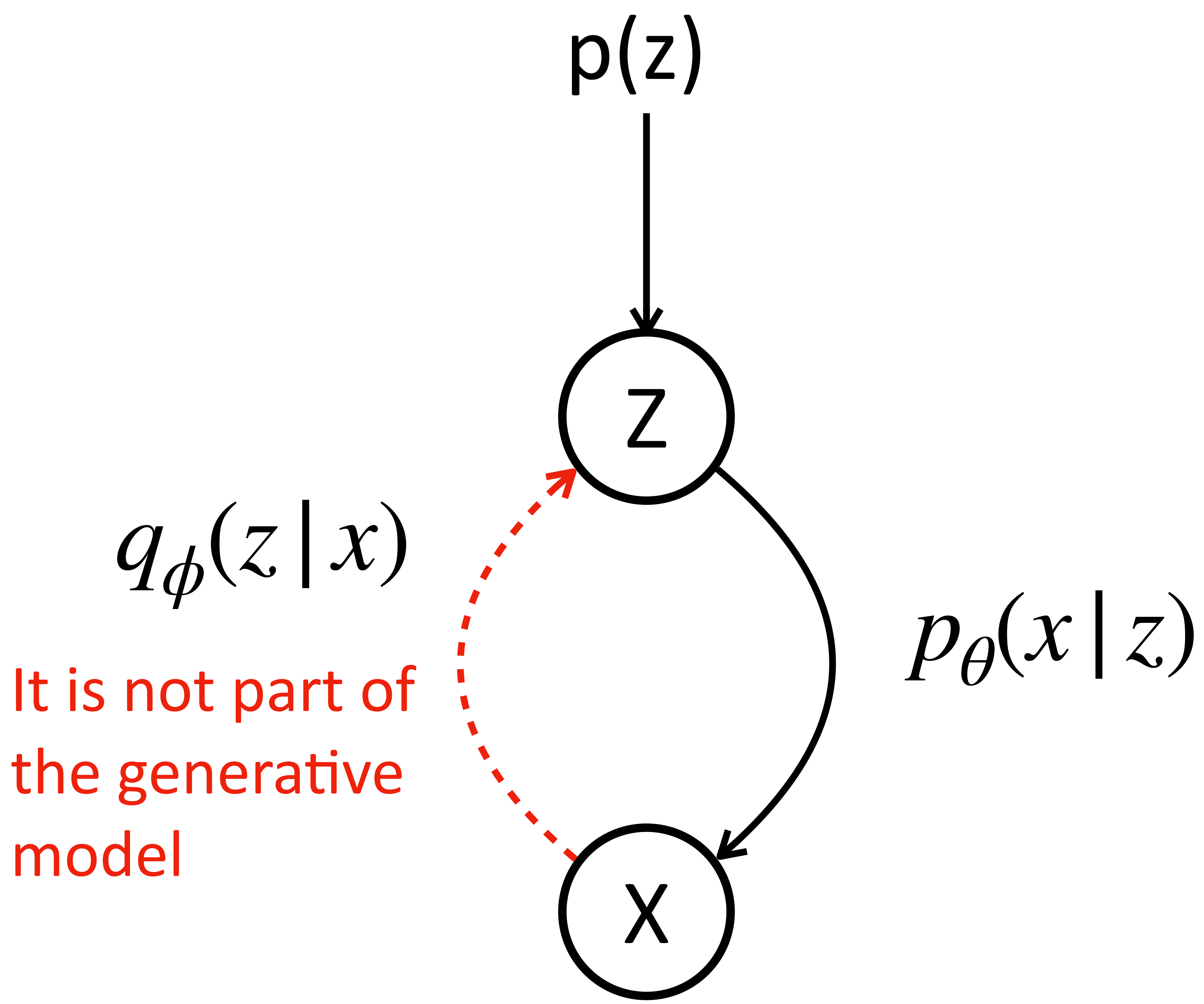

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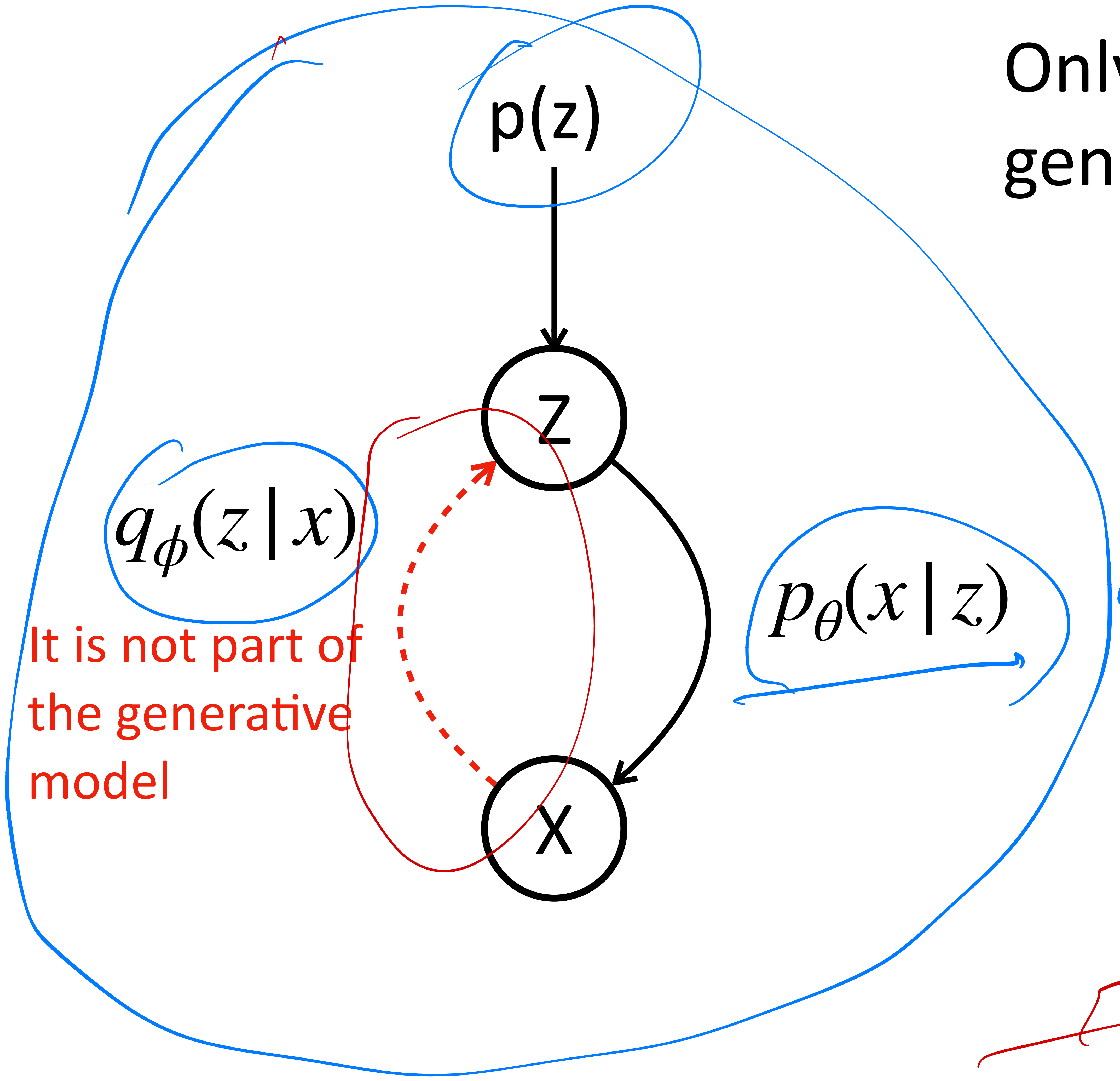
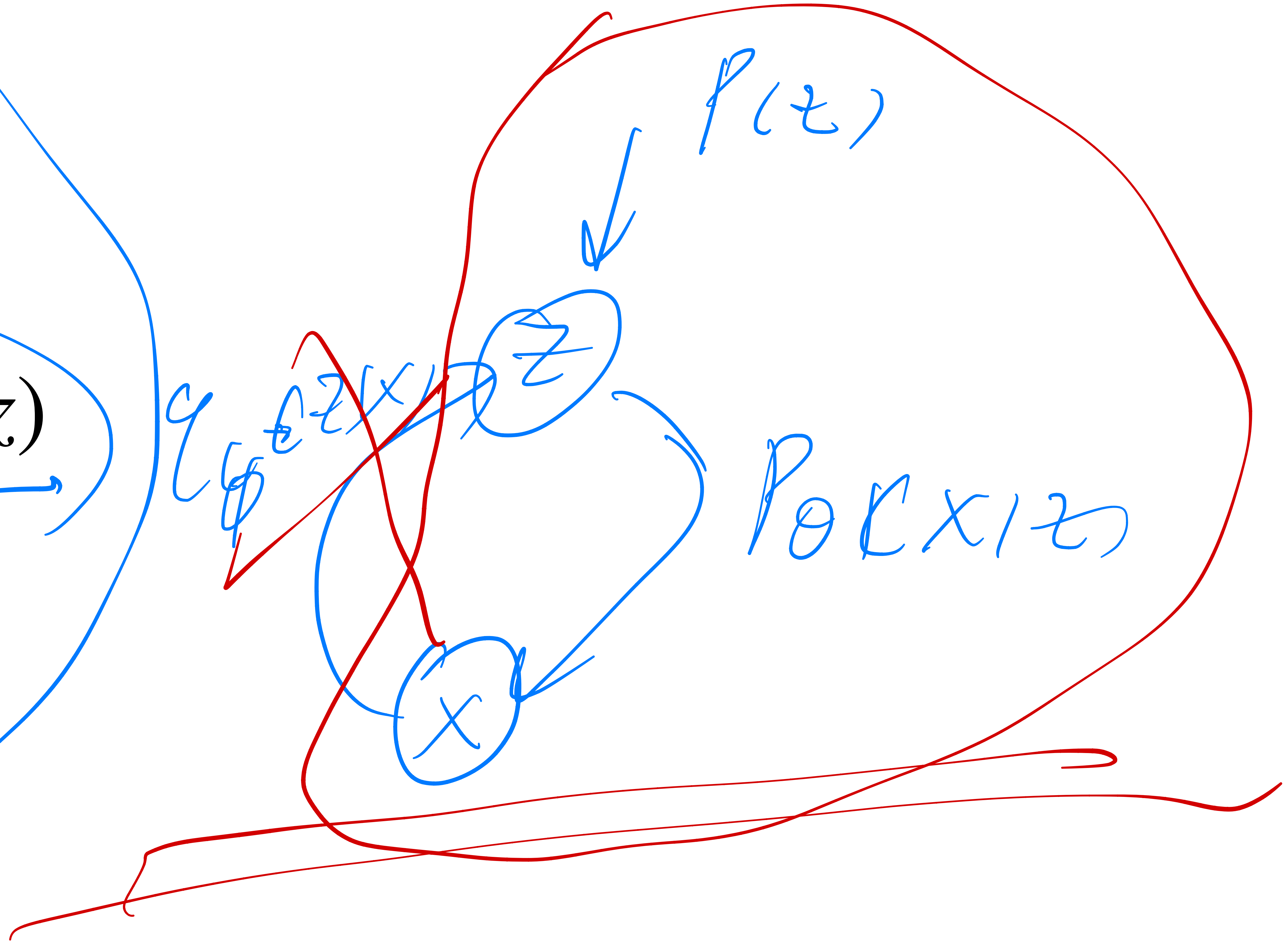


Only the right (black) part defines the generative model, and the distribution



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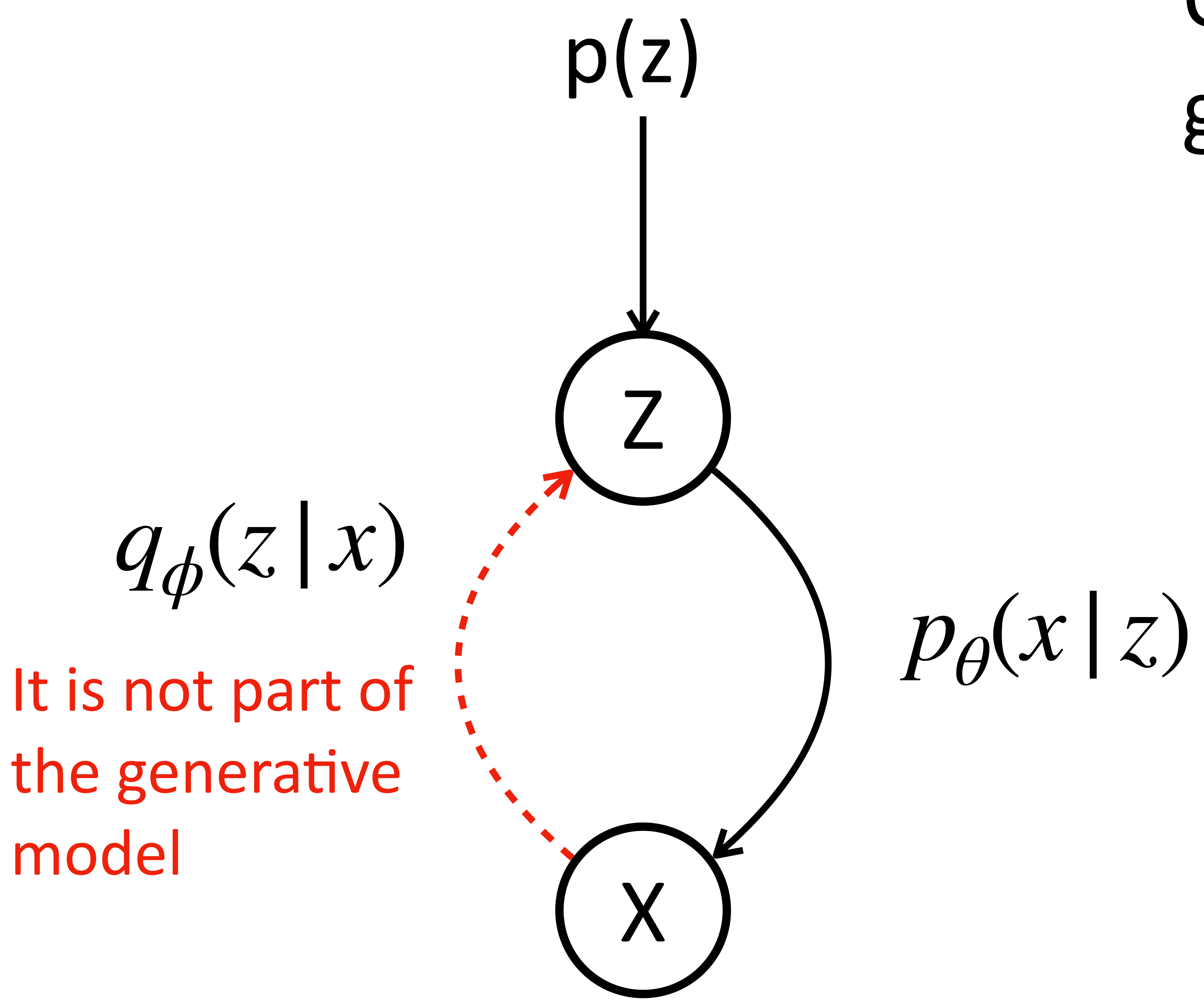

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$p_\theta(x\,|\,z)$: generative network/decoder

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

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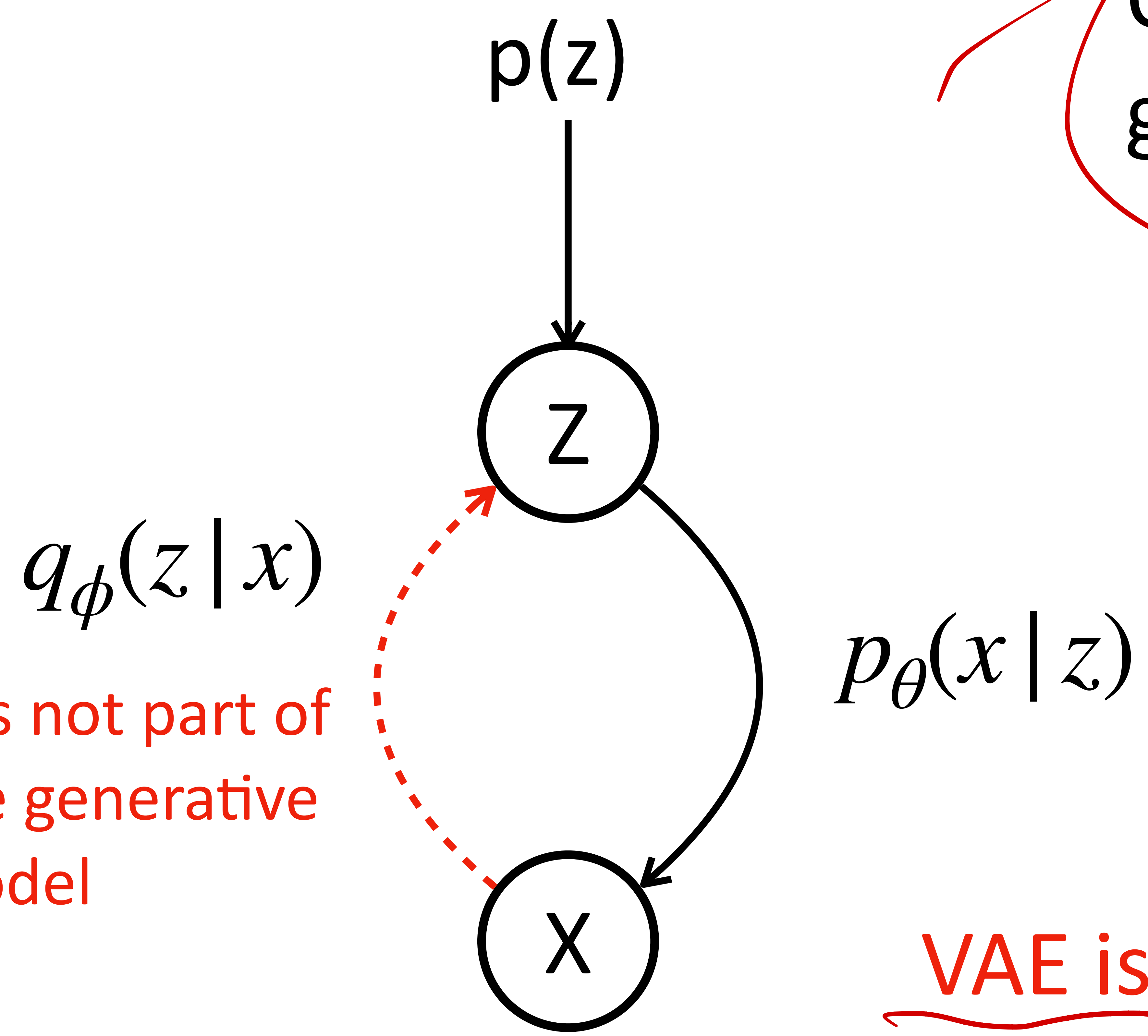

It is not part of the generative model

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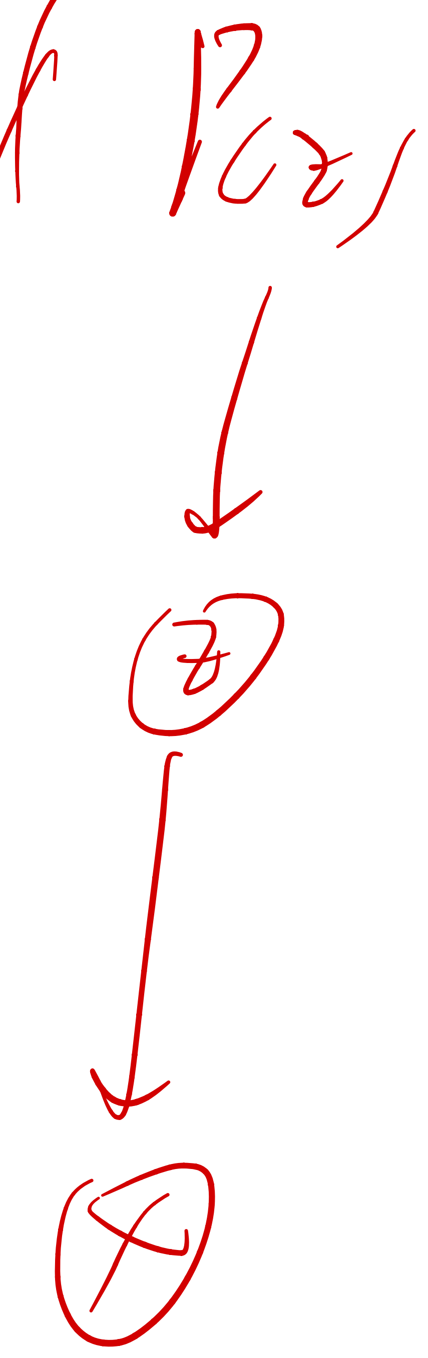

VAE is a name to represent both the model p(x) and the inference network that is used to train the model, but do not confuse them together

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 $p(\boldsymbol{\epsilon})$ $\rightarrow \mathcal{N}(0,1)$
  $\mathbf{g} \leftarrow \nabla_{\boldsymbol{\theta},\boldsymbol{\phi}} \widetilde{\mathcal{L}}^M(\boldsymbol{\theta}, \boldsymbol{\phi}; \mathbf{X}^M, \boldsymbol{\epsilon})$ (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 $(\boldsymbol{\theta}, \boldsymbol{\phi})$
return $\boldsymbol{\theta}, \boldsymbol{\phi}$

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E: ϕ → converge

M: θ

End-to-end, because the objectives are the same (ELBO)

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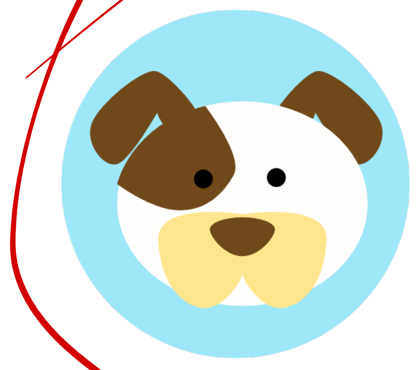
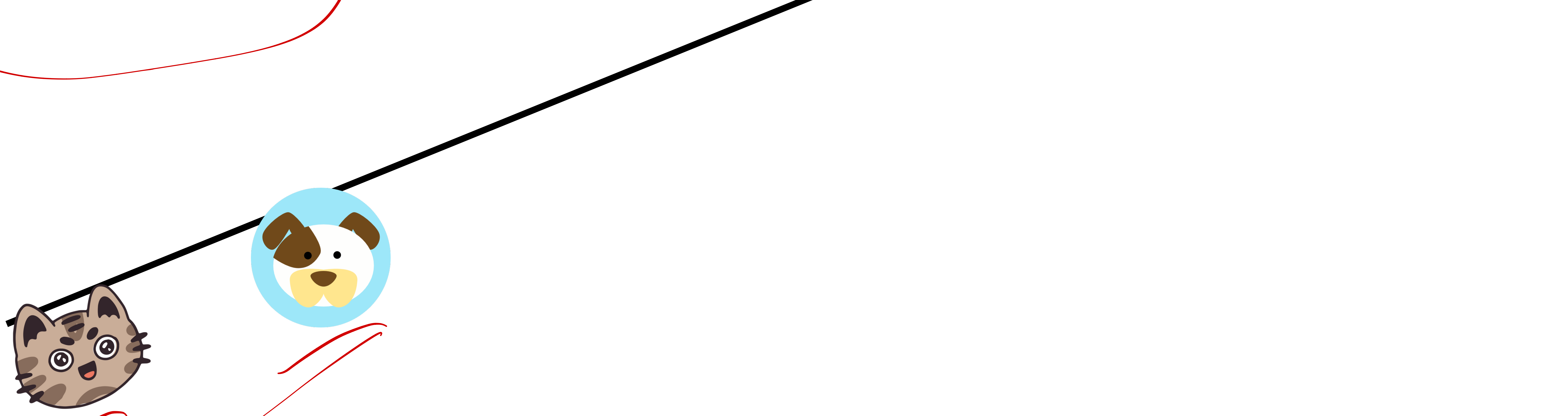
VAE training is optimizing ELBO with gradient descent

Recap: EM is Hill Climbing

 $\log p(x;\theta)$

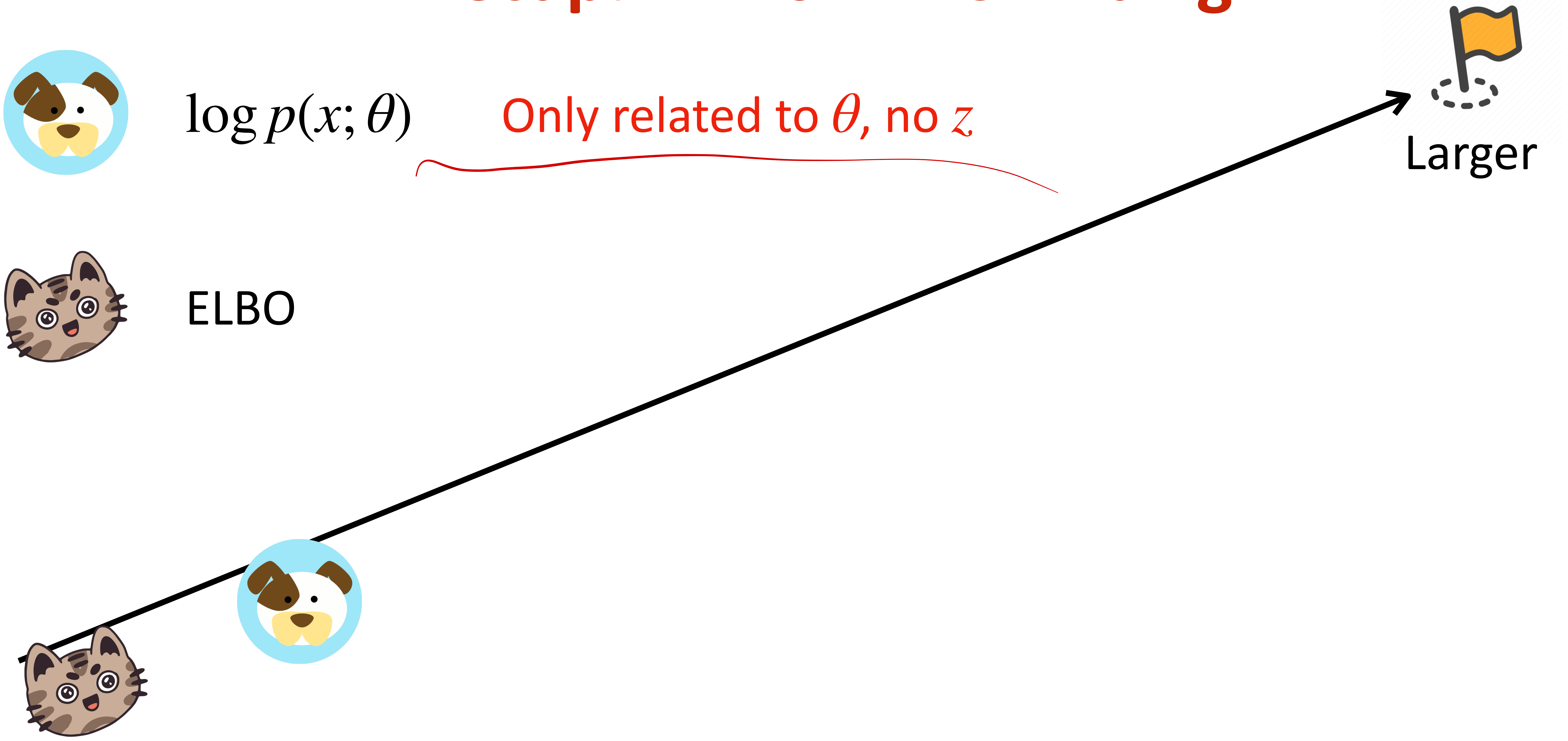
 ELBO



Recap: EM is Hill Climbing

$\log p(x;\theta)$ Only related to θ, no z

ELBO



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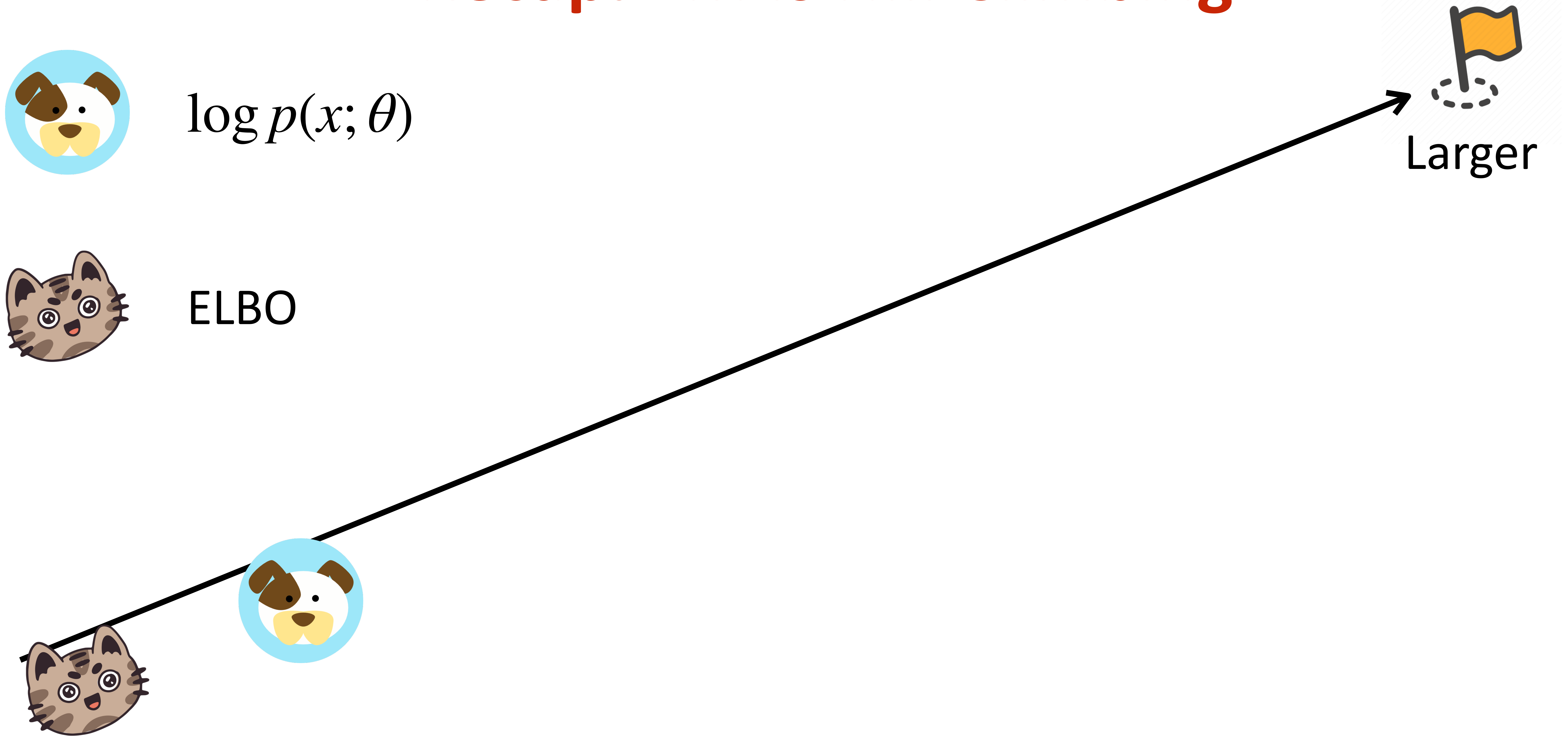

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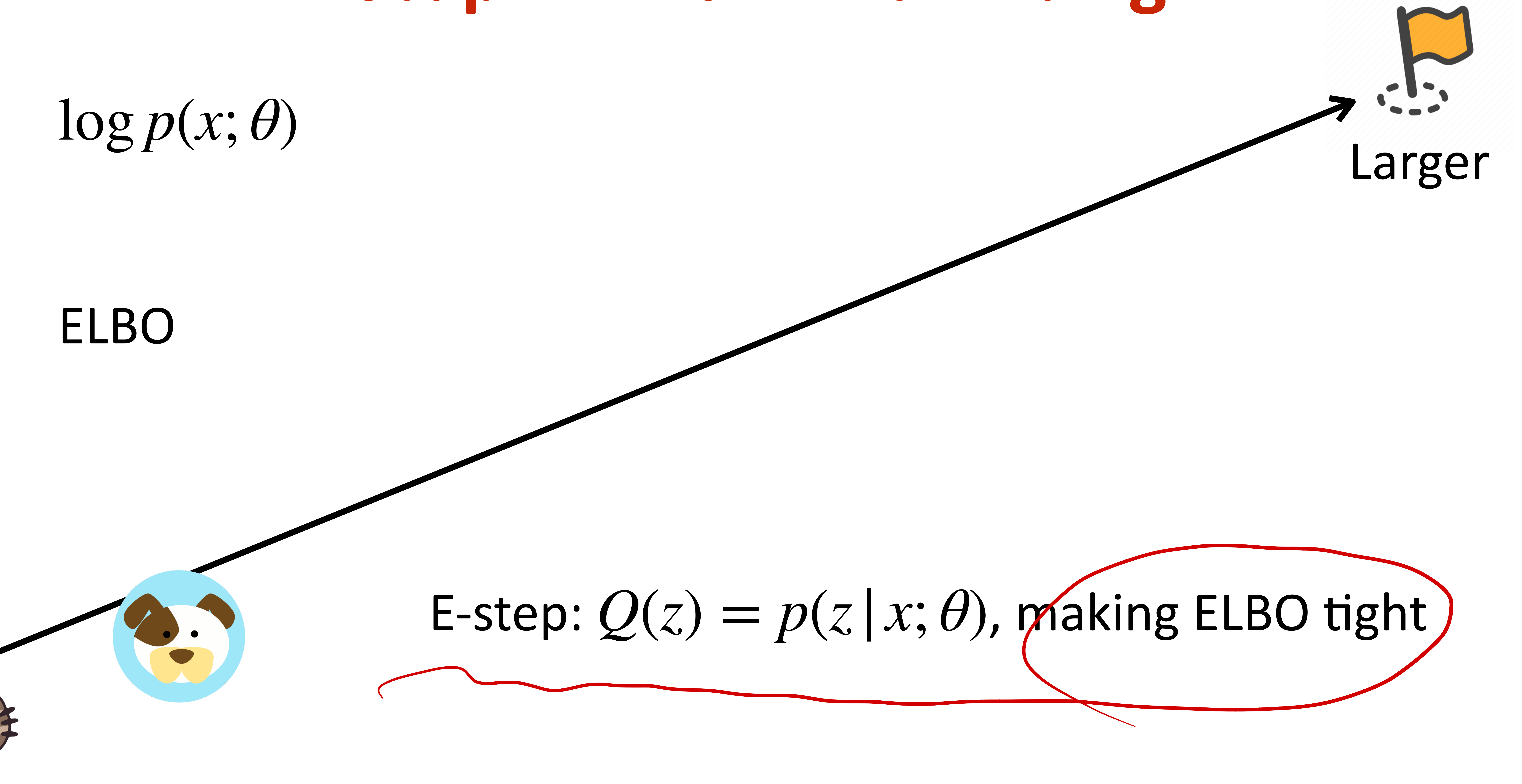

E-step: $Q(z) = p(z \mid x;\theta)$, making ELBO tight

Recap: EM is Hill Climbing

$\log p(x;\theta)$

ELBO

Larger

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

“dog” doesn’t change, because θ does not change

Recap: EM is Hill Climbing

$\log p(x;\theta)$

ELBO

Larger

cat dog

cat dog

ϕ θ

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$\log p(x)$ ↑

Recap: EM is Hill Climbing

$\log p(x;\theta)$

ELBO

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

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

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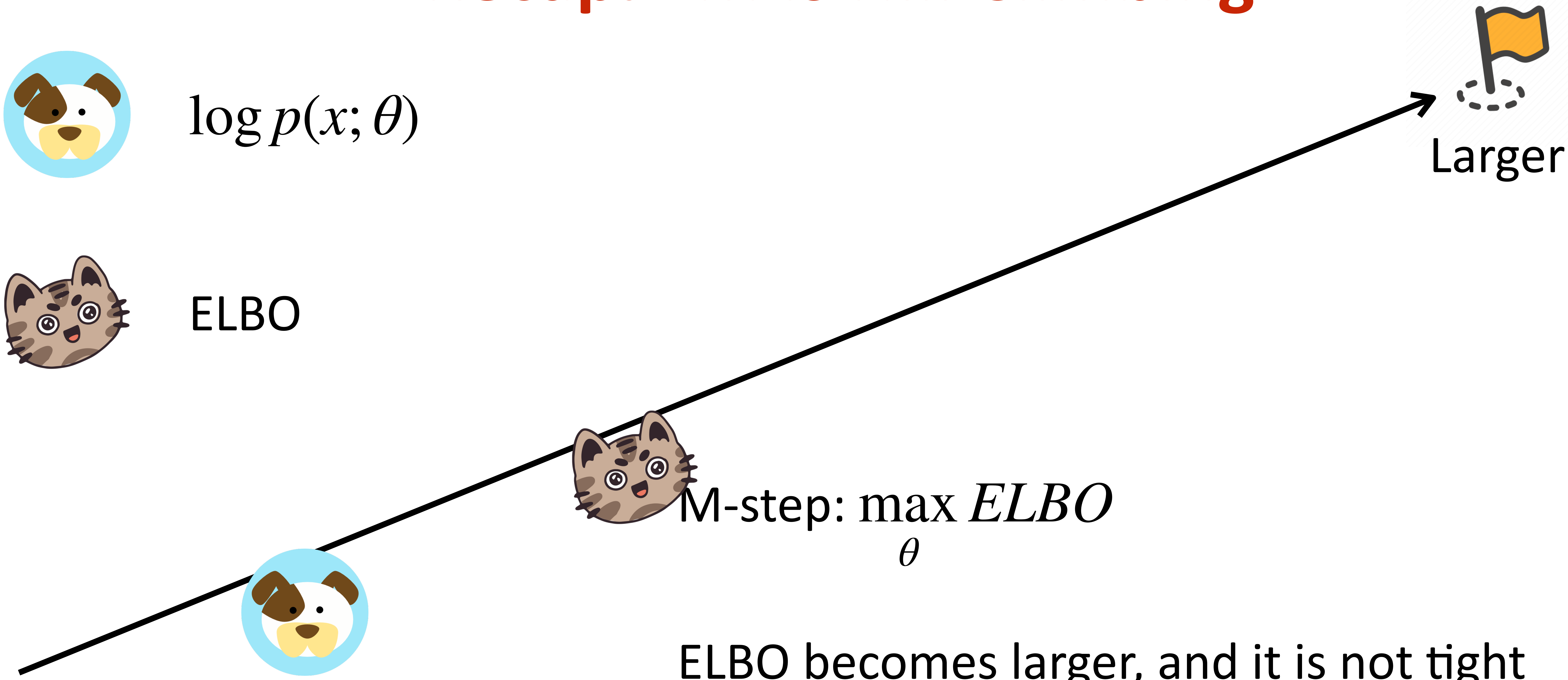

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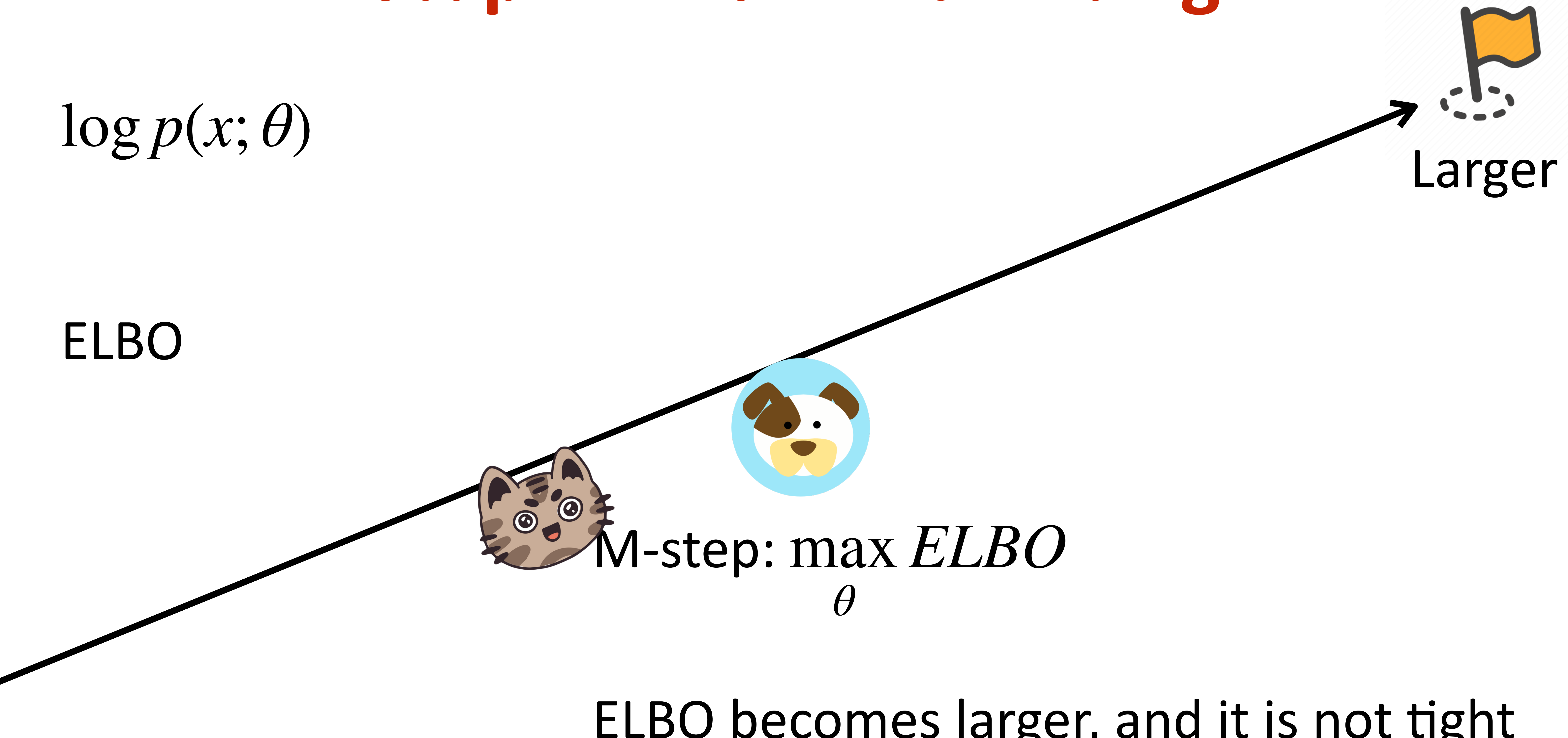

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Is VAE training still Hill Climbing?

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In VAE training, there is no guarantee that $\log p(x)$ is monotonically increasing

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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, $q_{\phi}(z\,|\,x) = p(z)$ and z and x becomes independent (especially in applications of NLP)

$q(z|x)$ $\qquad$ $z \perp x$

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Z does not affect x, the model degenerates to a generative model without latent variables

z

x

The Posterior Collapse Issue

$q_\phi(z|x)$

$\rightarrow p(z)$

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Researchers commonly blame that the KL regularizer is too strong for this and use a weight $0 < \lambda < 1$ to control it:

The Posterior Collapse Issue

MLE

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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?

E-Step:

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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

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

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LAGGING INFERENCE NETWORKS AND POSTERIOR COLLAPSE IN VARIATIONAL AUTOENCODERS

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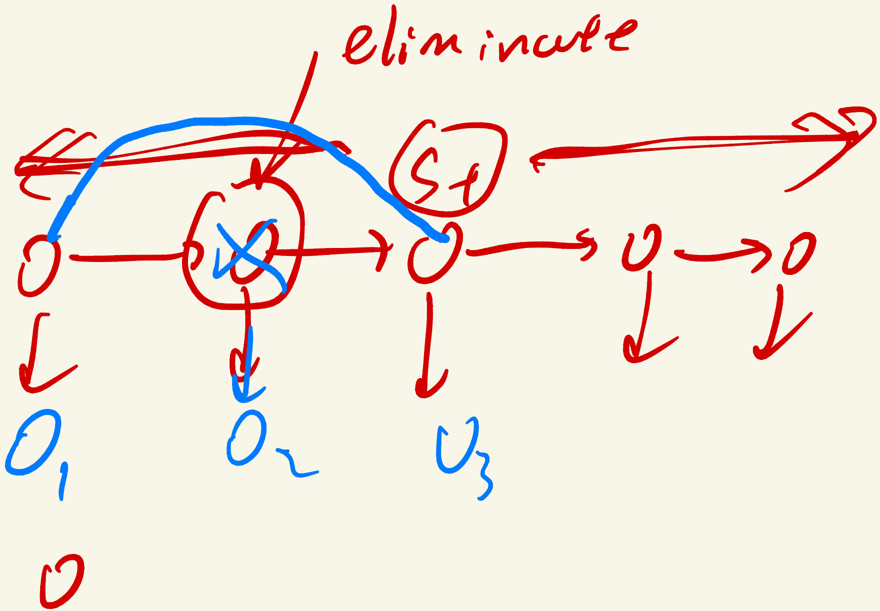
AutoEncoders



eliminate
S_t
O_1
O_2
O_3

AutoEncoders

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

AutoEncoders

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AE: $$\log p_{\theta}(x \mid q(x))$$

AutoEncoders

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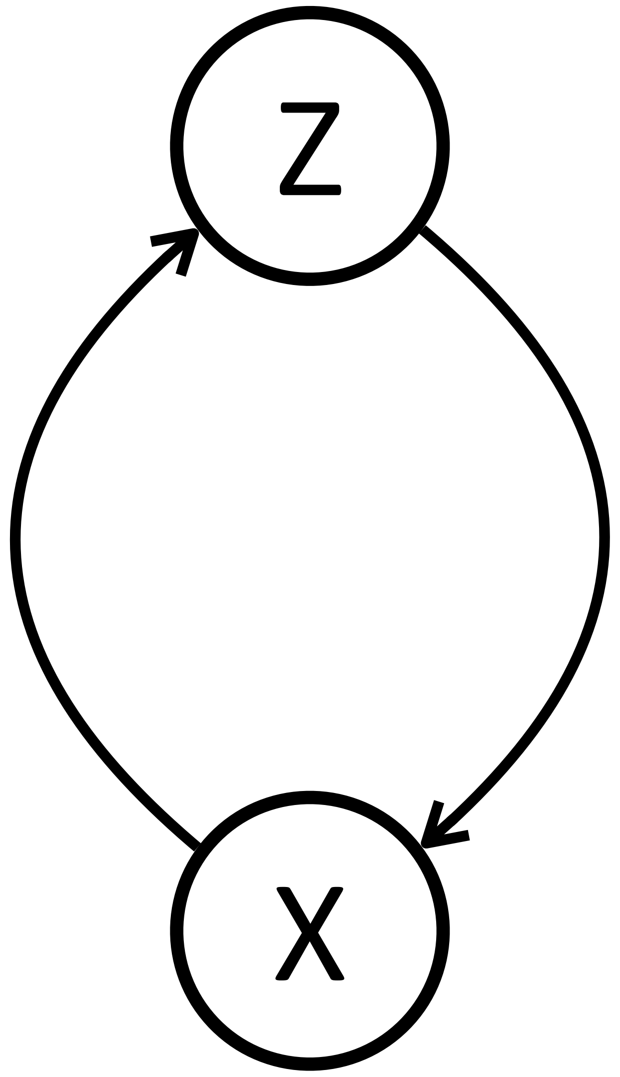

AutoEncoders

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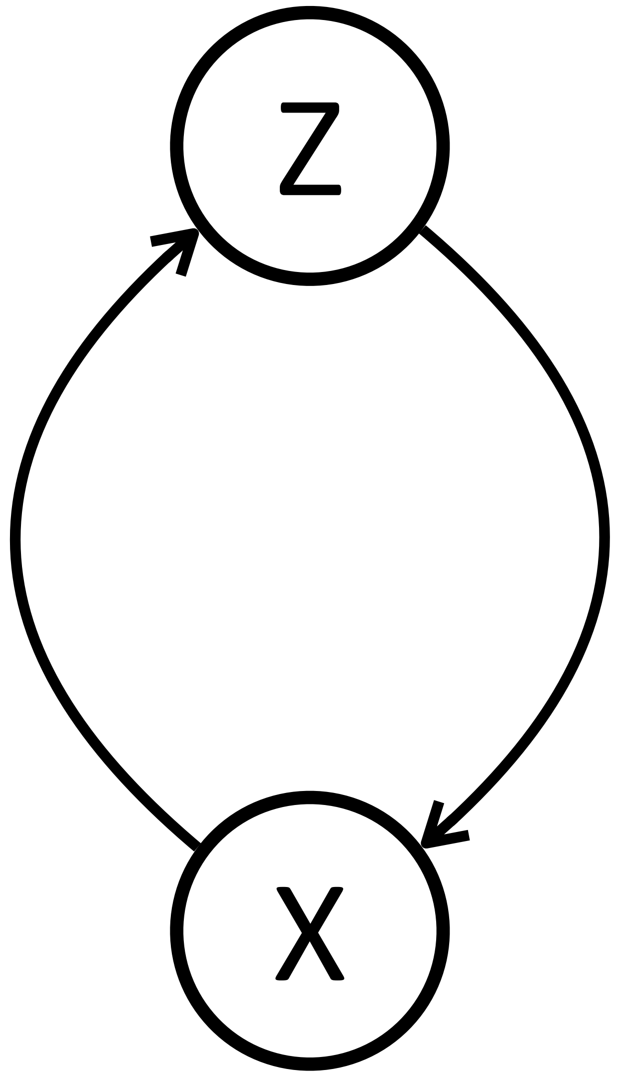
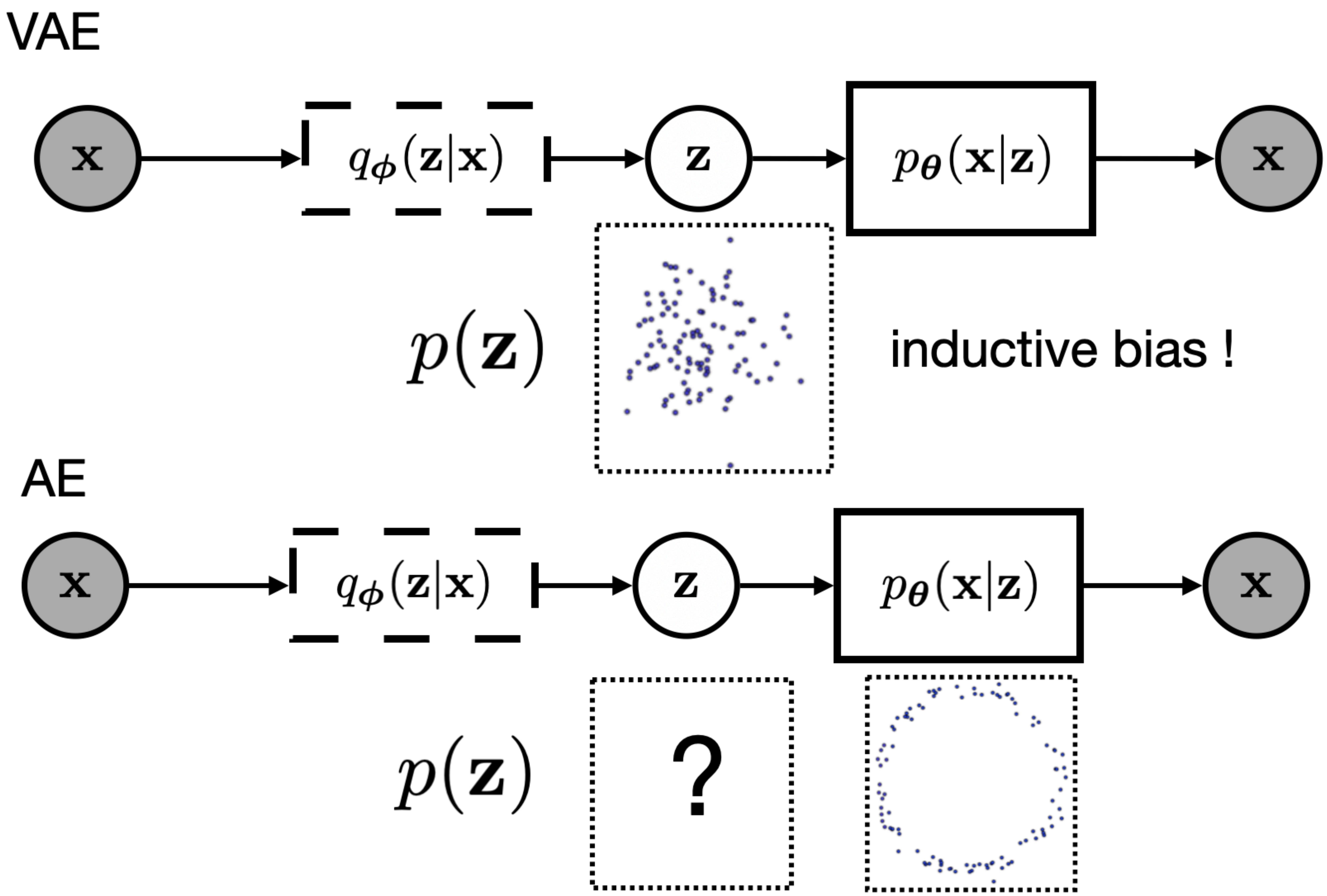


1. Can we generate X samples from an autoencoder?
2. Can we approximate p(x) given x with an autoencoder?
3. What is the difference between the representation space from AE and VAE?

VAE v.s. AE


VAE
$\mathbf{x}$
$q_\phi(\mathbf{z}|\mathbf{x})$
$\mathbf{z}$
$p_\theta(\mathbf{x}|\mathbf{z})$
$\mathbf{x}$
$p(\mathbf{z})$
inductive bias !
AE
$\mathbf{x}$
$q_\phi(\mathbf{z}|\mathbf{x})$
$\mathbf{z}$
$p_\theta(\mathbf{x}|\mathbf{z})$
$\mathbf{x}$
$p(\mathbf{z})$
?

Generative Adversarial Nets

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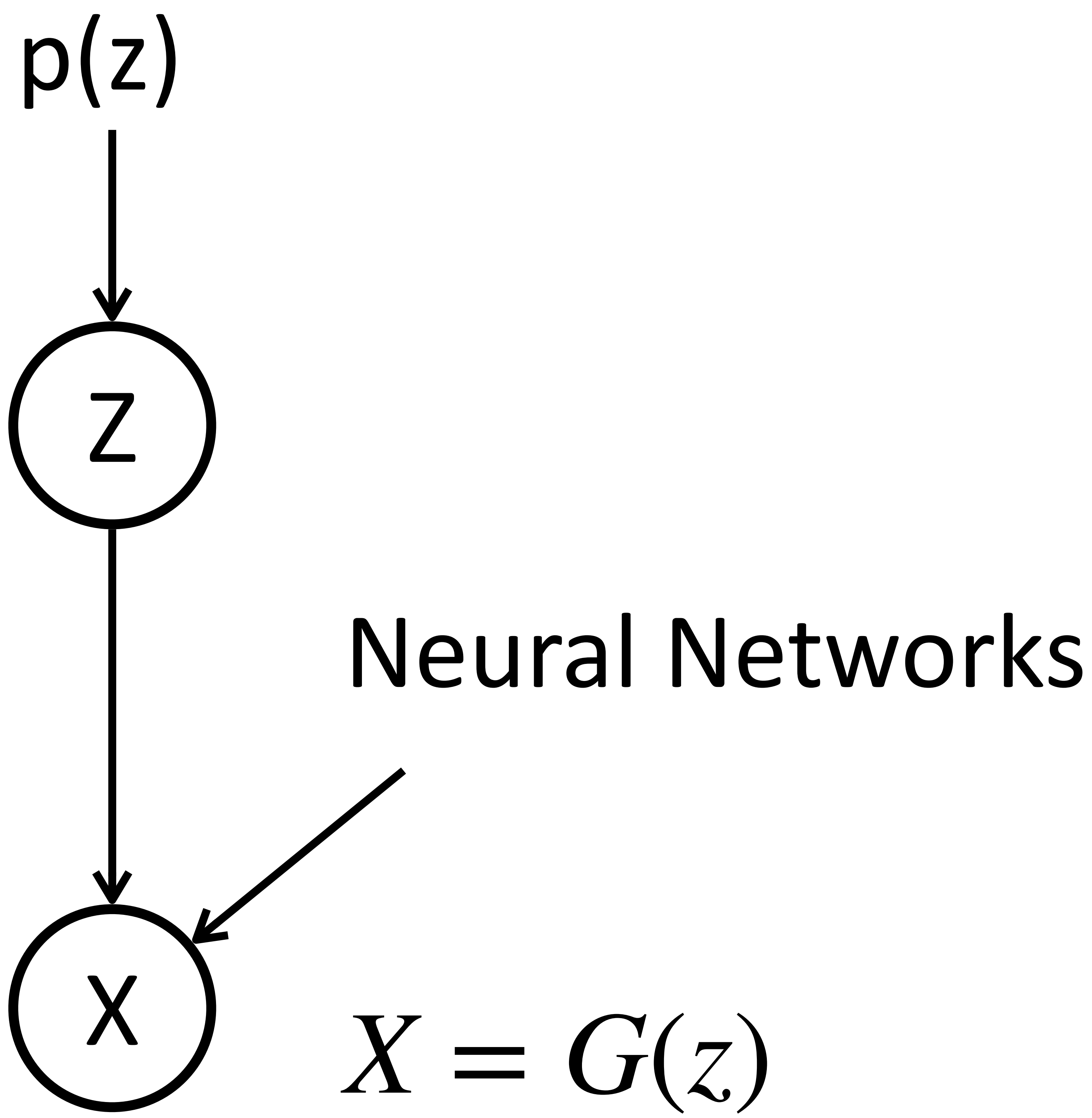
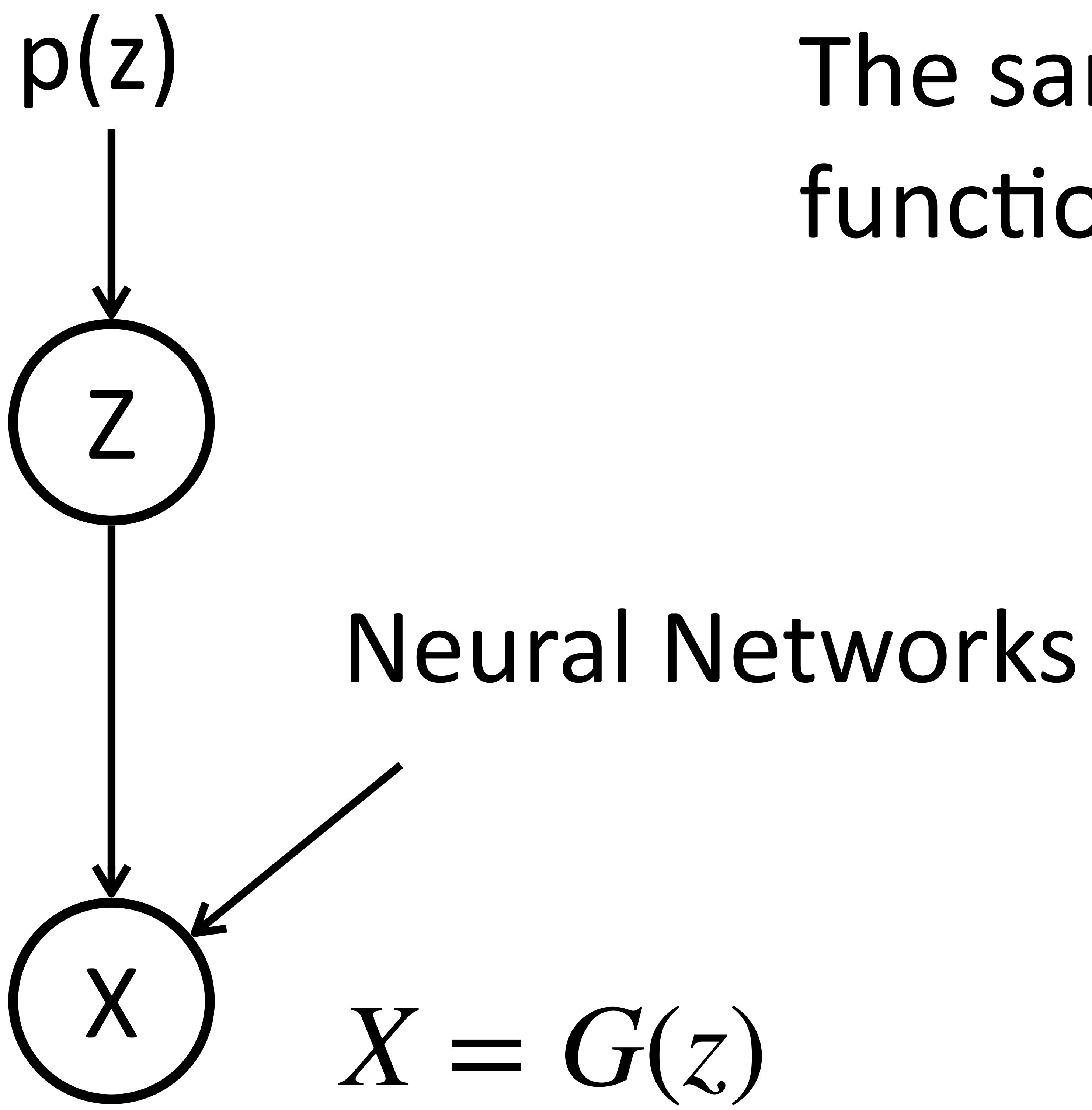
Generative Adversarial Networks

The GAN Model



$$X = G(z)$$

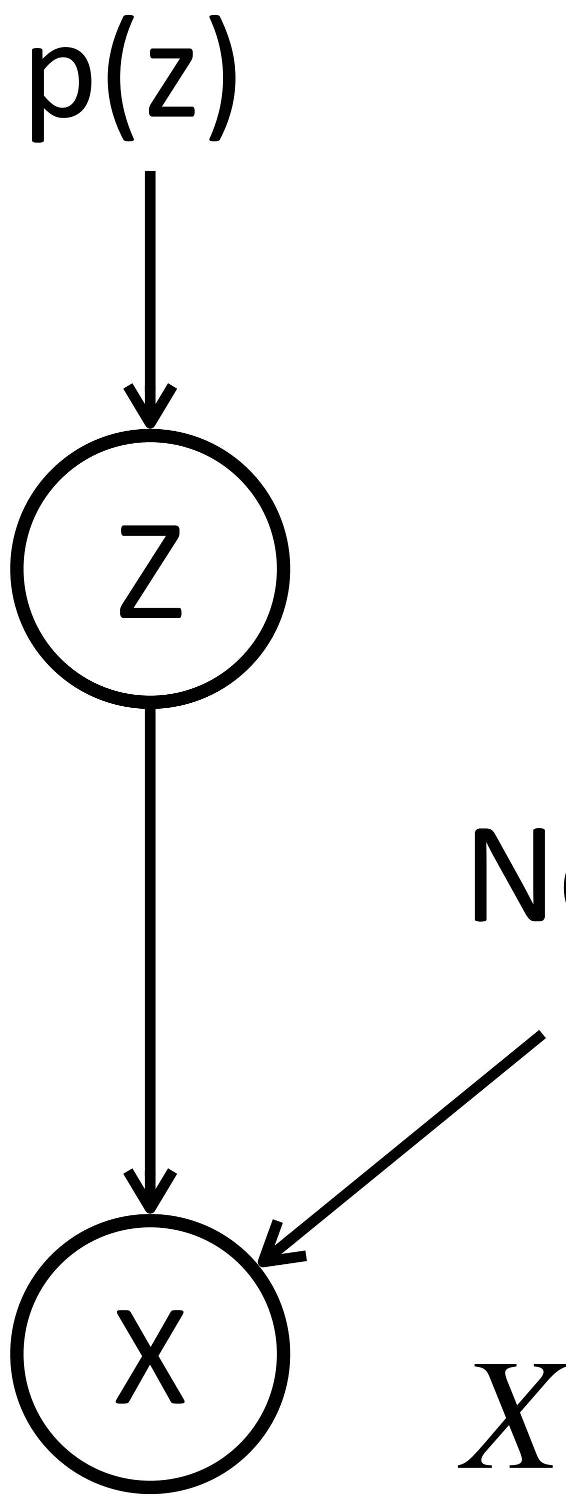
The GAN Model



$$X = G(z)$$

The same as the VAE model, except that x is a deterministic function of z, but it can be a distribution as well

The GAN Model



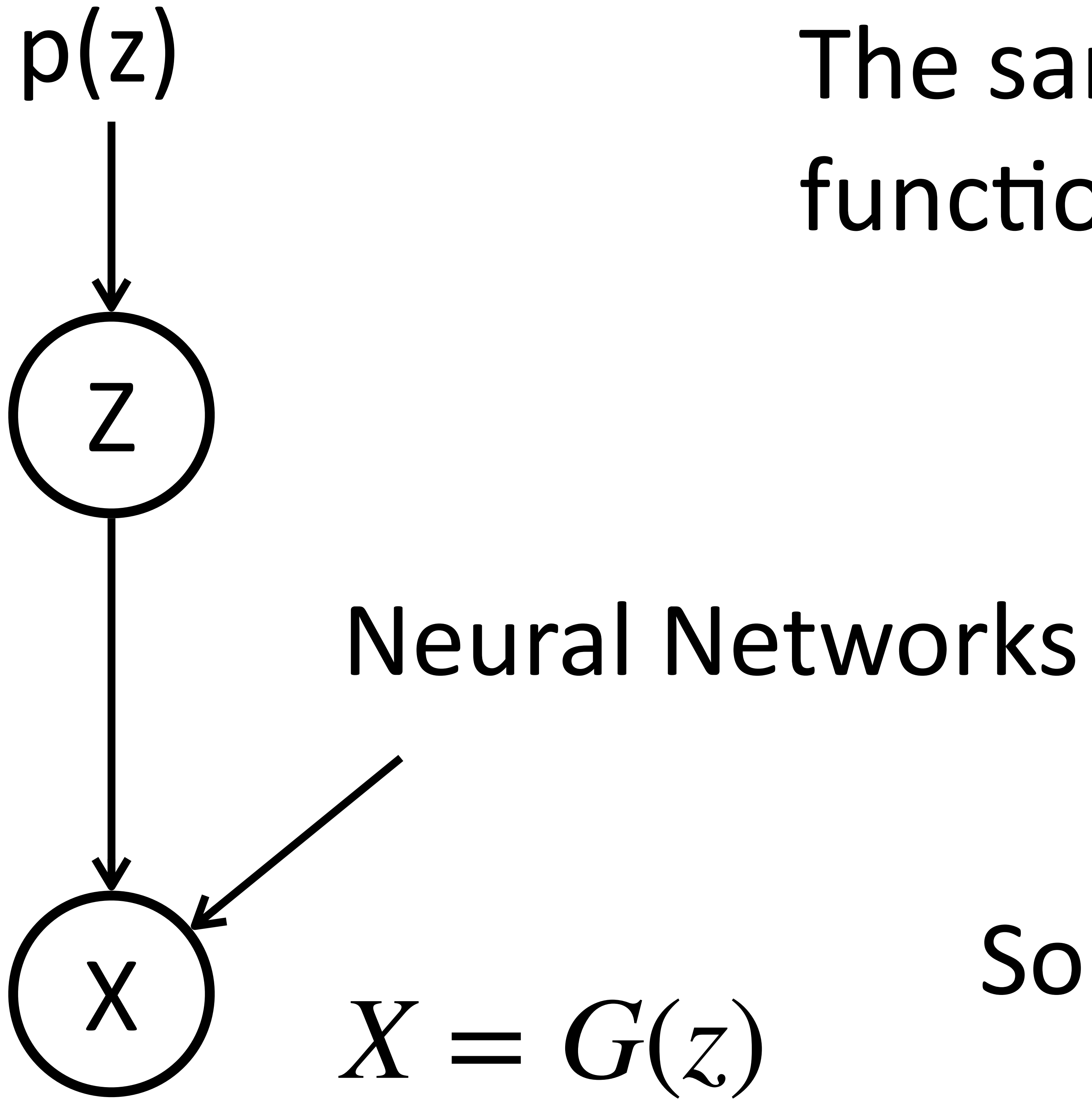
Neural Networks

$$X = G(z)$$

The same as the VAE model, except that x is a deterministic function of z, but it can be a distribution as well

Can VAE use a deterministic x = G(z)?

The GAN Model



$$X = G(z)$$

The same as the VAE model, except that x is a deterministic function of z, but it can be a distribution as well

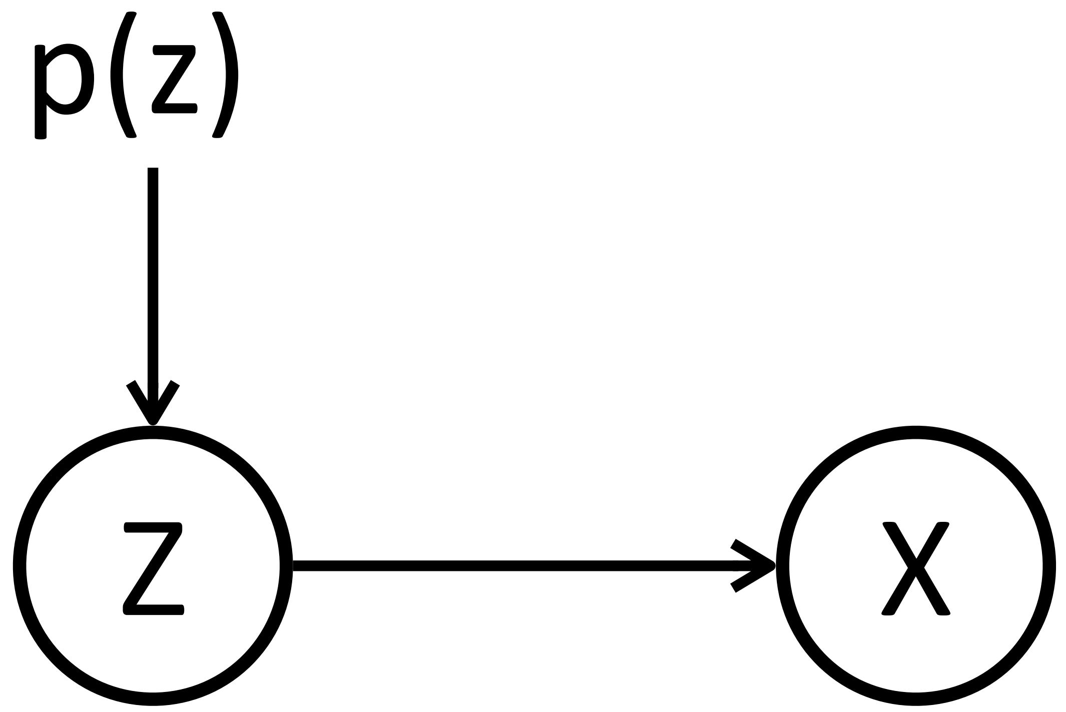
Can VAE use a deterministic x = G(z)?

Sometimes we call GANs *implicit* generative models

You can draw samples, but hard to evaluate p(x)

Training GANs

Computation Graph



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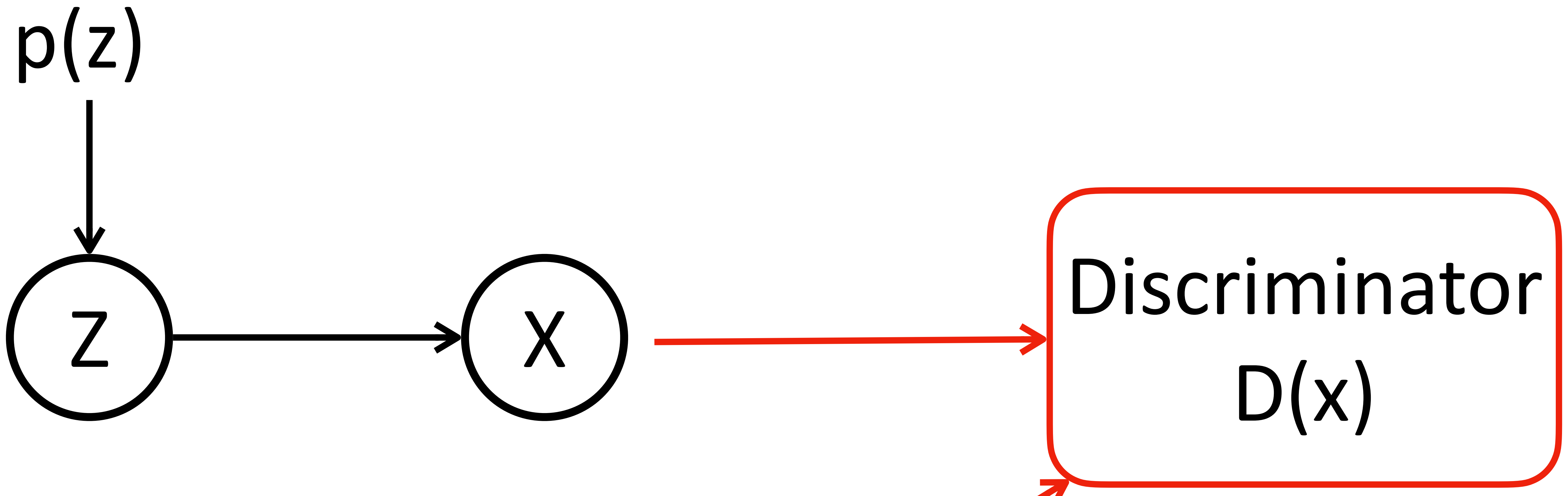

$$X = G(z)$$

$$x \sim p_{data}(x)$$

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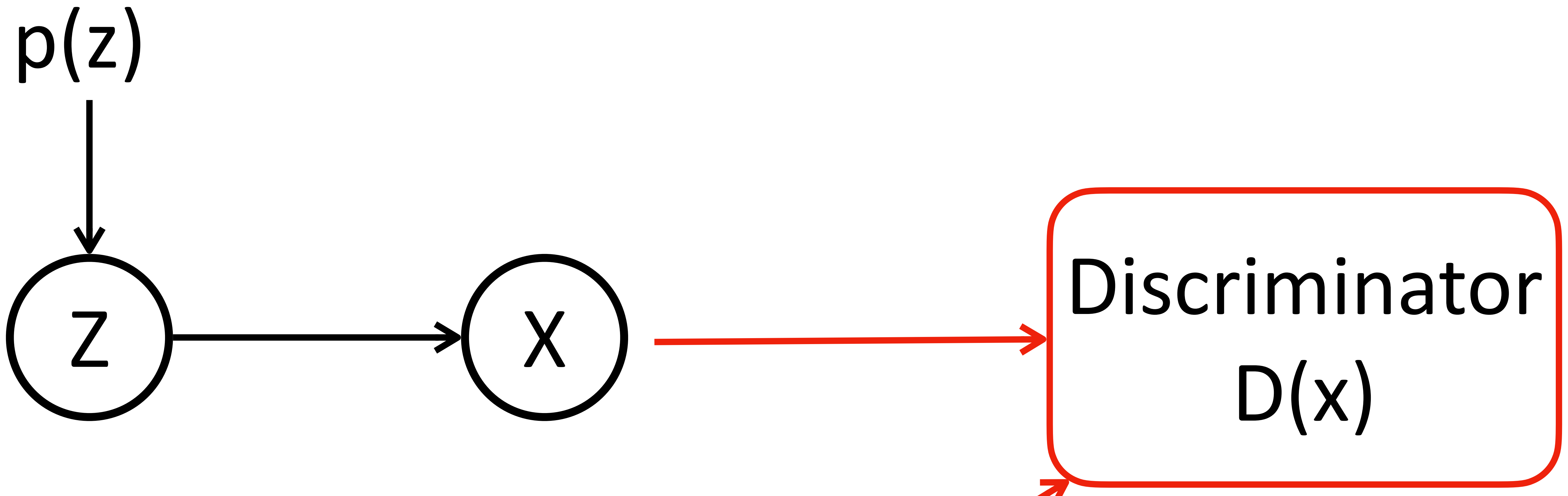

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Discriminate whether the input is real or fake

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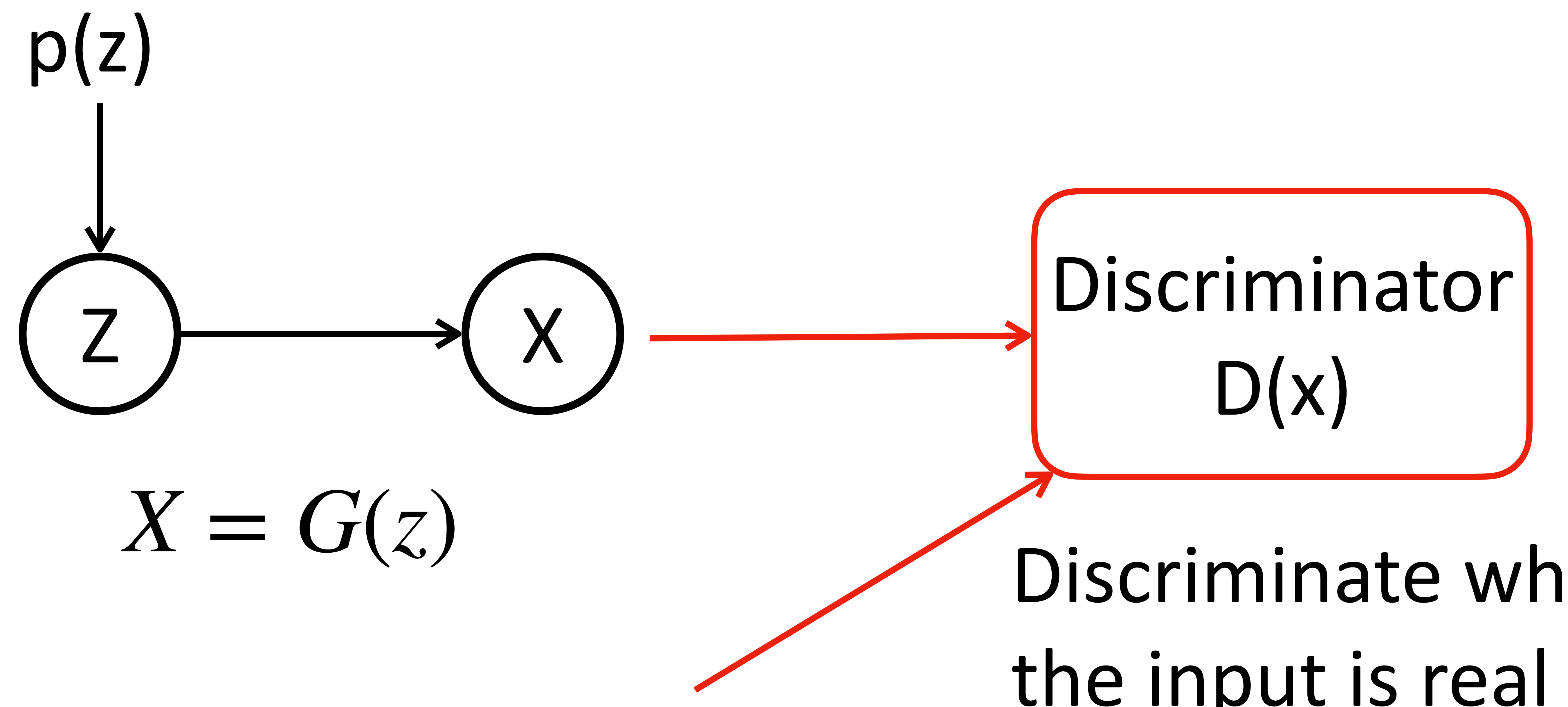

$$X = G(z)$$

$$x \sim p_{data}(x)$$

Discriminate whether the input is real or fake

1. Generator is trained to produce realistic examples to fool the discriminator

Training GANs

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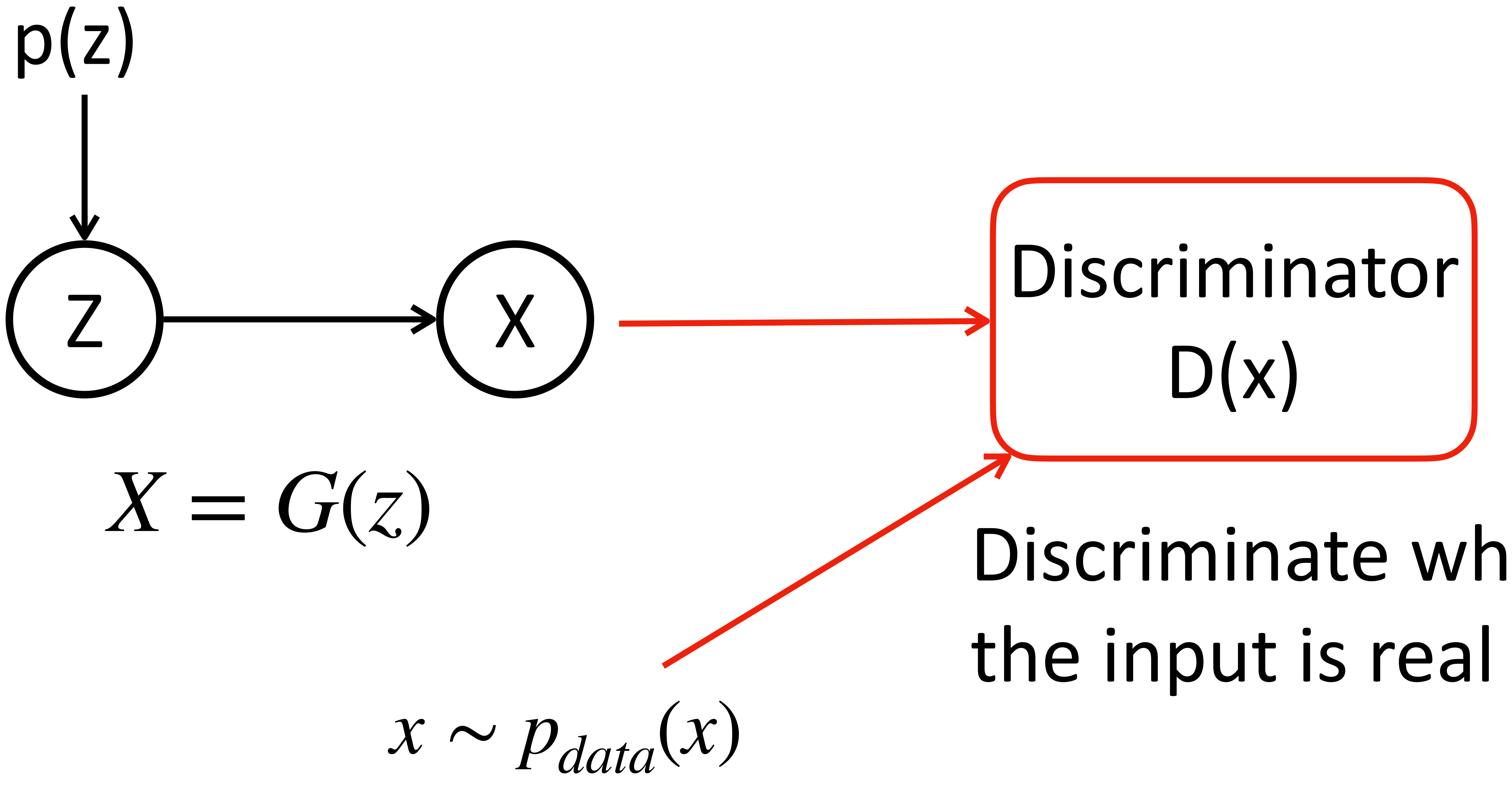

Discriminate whether the input is real or fake

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2. Discriminator is trained to discriminate real and fake examples

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The two objectives are against each other

Adversarial Game

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Adversarial Game

$$\min_G \max_D V(D, G) = \mathbb{E}_{\boldsymbol{x} \sim p_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z} \sim p_{\boldsymbol{z}}(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z})))].$$

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Classification loss

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Classification loss

G(z) is trained to minimize the probability of G(z) recognized as “fake” by D

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Classification loss

G(z) is trained to minimize the probability of G(z) recognized as “fake” by D

D(x) is trained with a standard classification loss

Training GANs

1. GAN is a new algorithm to train a common generative model (VAE as well)

2. GAN training is not MLE