香港科技大學
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UNIVERSITY OF SCIENCE
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COMP 5212
Machine Learning
Lecture 21

Variational Autoencoders

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Auto-Encoding Variational Bayes

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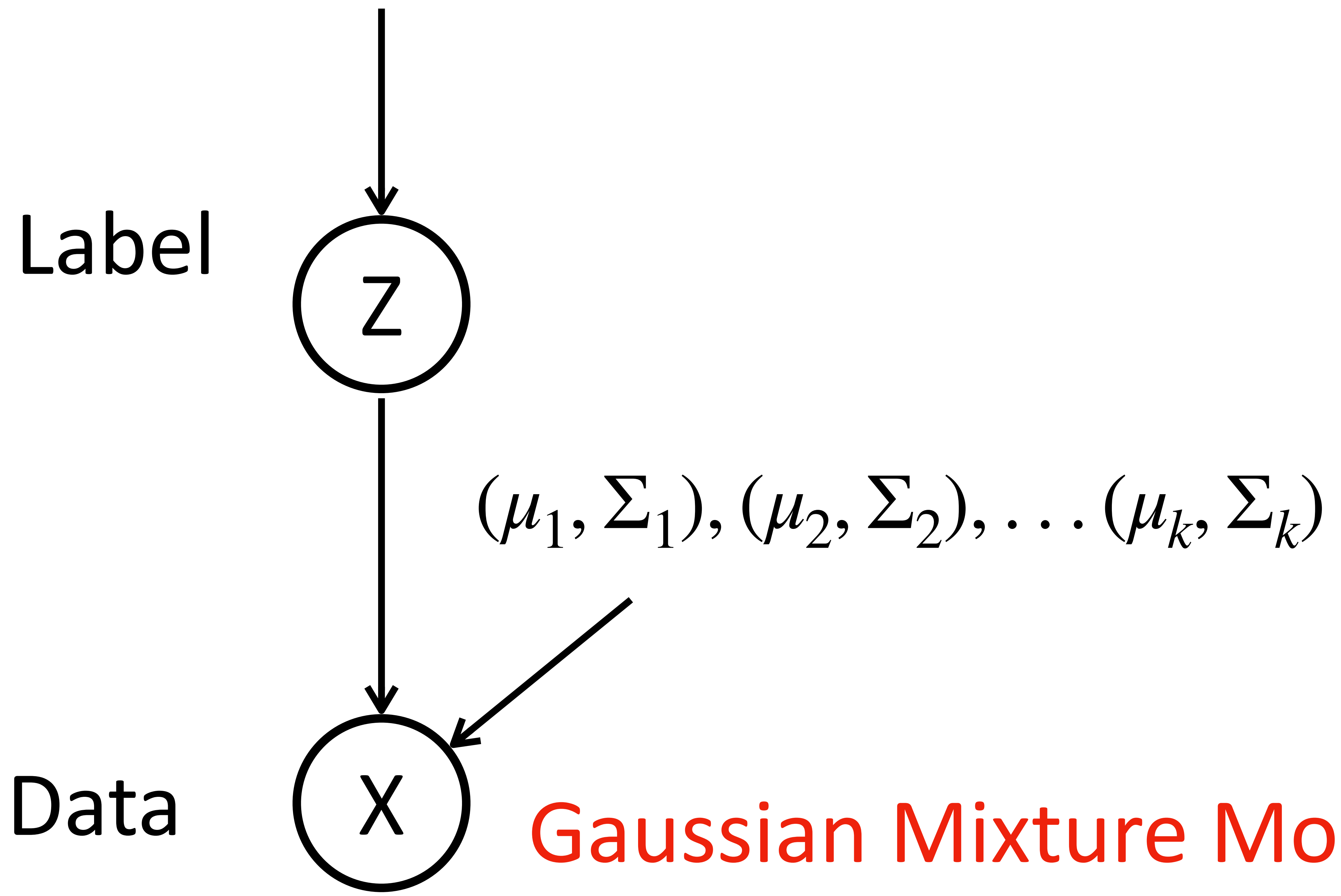
The first test-of-time award in ICLR

VAE is a Generative Model

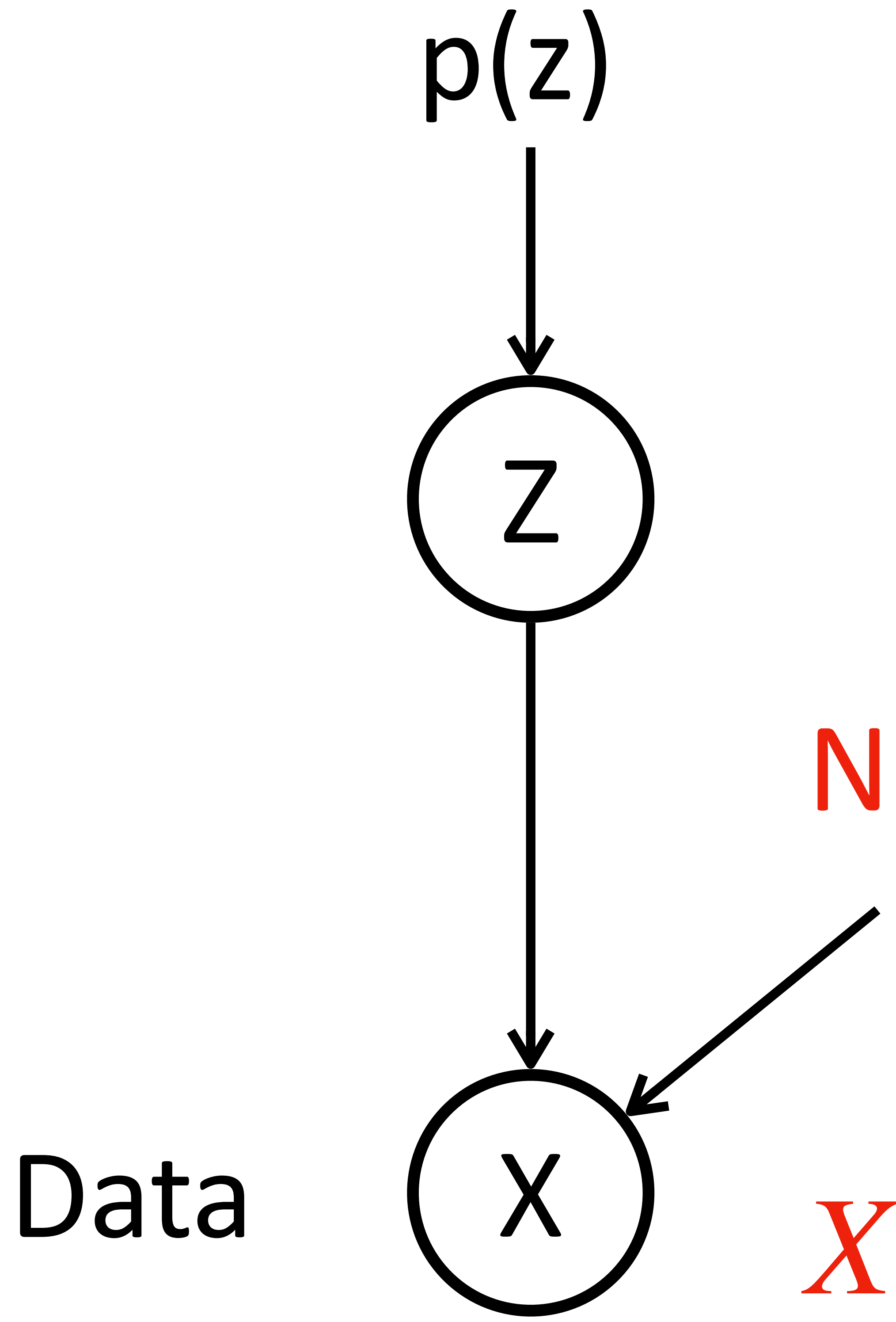
p(z): multinomial , k
classes(e.g. uniform)



Gaussian Mixture Model (GMM)

The VAE Model

p(z) is a normal distribution in most cases

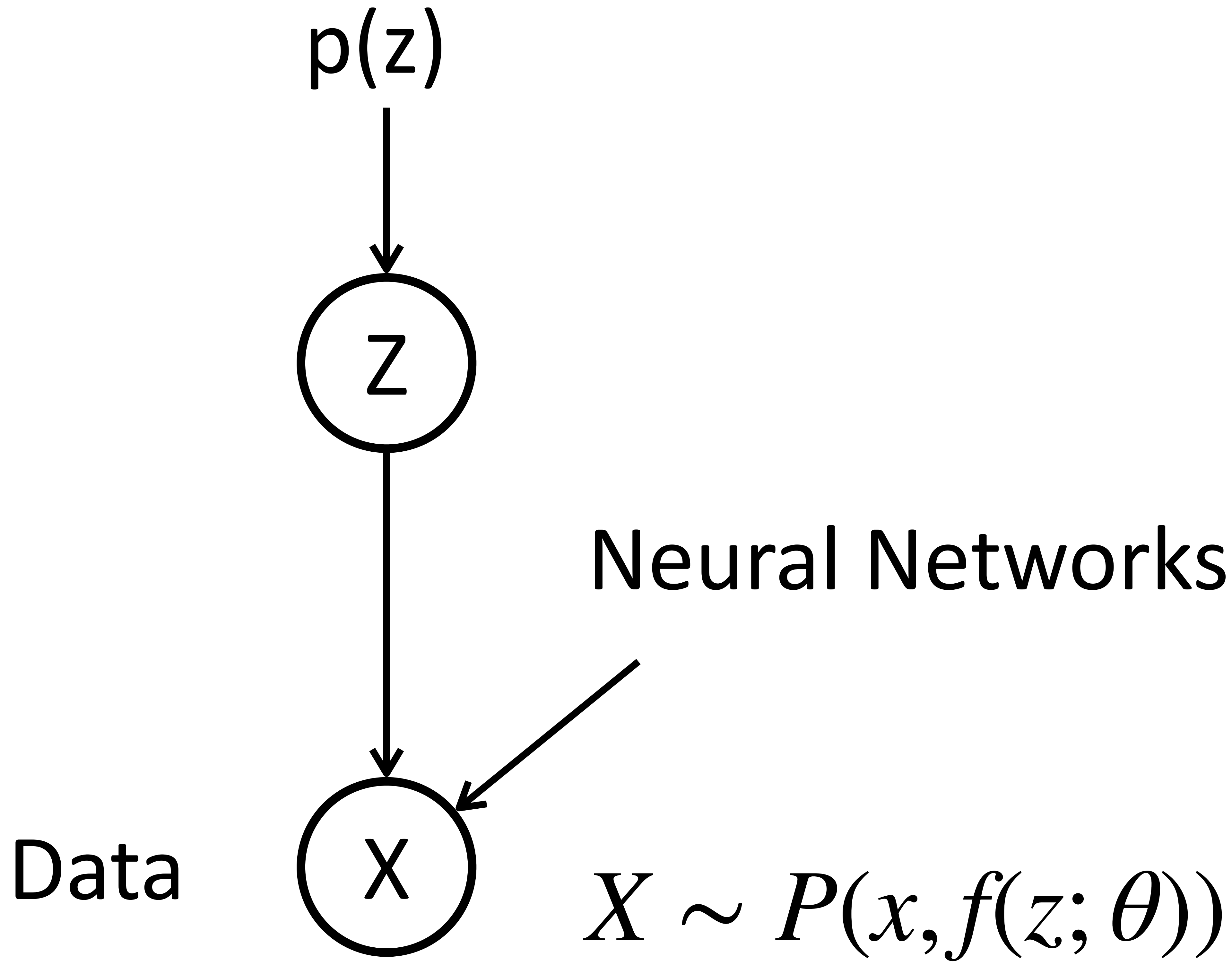


Neural Networks

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

f is a neural network taking Z as input

Training

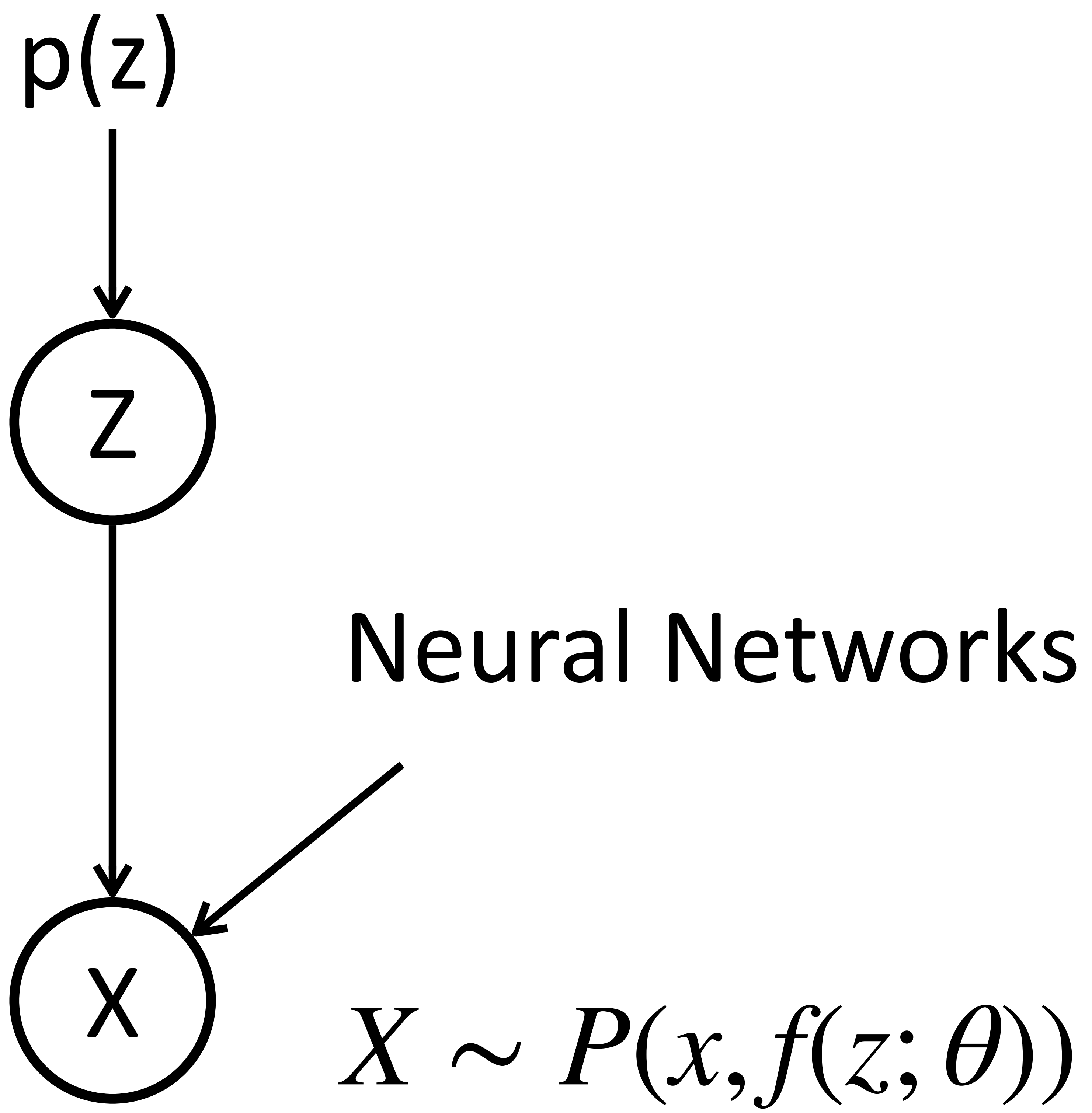


$$X \sim P(x, f(z;\theta))$$

How to train the model? Can we do MLE?

Intractable P(X), EM algorithm?

Let's try EM



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

E-Step: compute P(z|x)

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

This is ok?

M-Step: the ELBO objective

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

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)

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

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)

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

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

Variational Inference

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:

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

Same objective, different parameters to optimize

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

Training VAEs

E-Step:

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

Can we do gradient descent over ϕ?

M-Step:

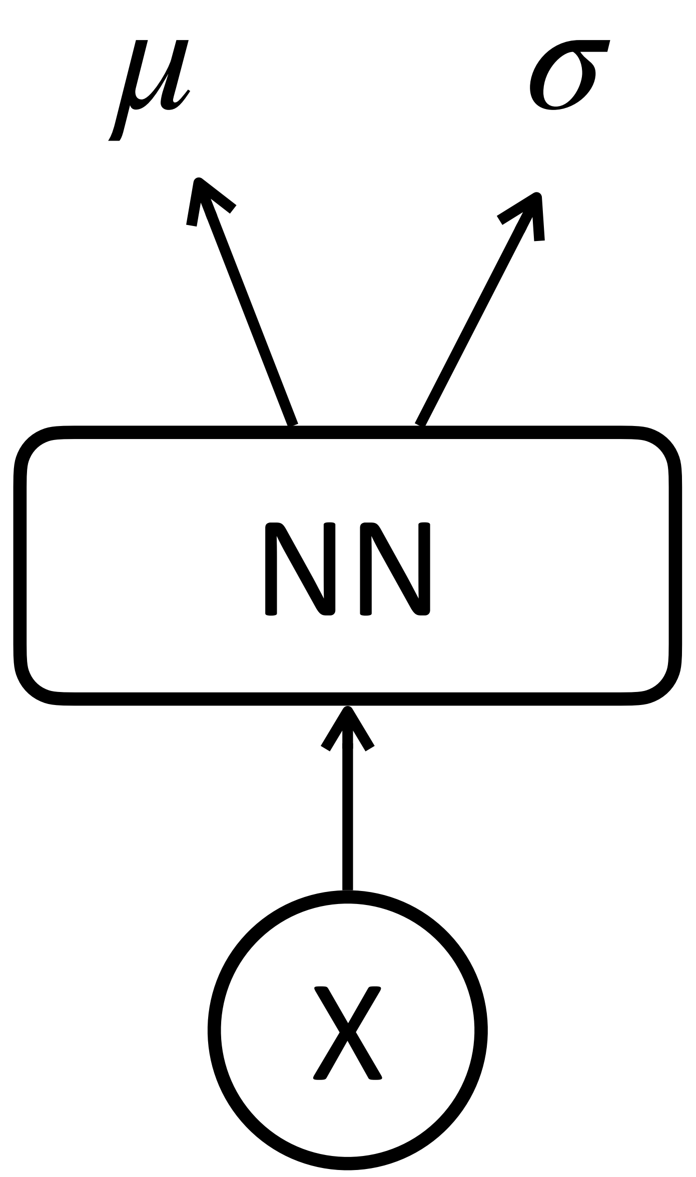
$$\text{argmax}_{\theta} \sum_{z} q(z|x;\phi) \log \frac{p(x,z;\theta)}{q(z|x;\phi)}$$

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

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

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

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



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:

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

Same objective, different parameters to optimize

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

Training VAEs

E-Step:

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

Can we do gradient descent over ϕ?

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

Reparameterization Trick

E-Step:

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

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?

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

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

Can you verify z in this equation is Gaussian?

Reparameterization Trick

E-Step:

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

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

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

1. Tractable inverse CDF. In this case, let $\boldsymbol{\epsilon} \sim \mathcal{U}(\mathbf{0}, \mathbf{I})$, and let $g_{\boldsymbol{\phi}}(\boldsymbol{\epsilon}, \mathbf{x})$ be the inverse CDF of $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$. 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 $\boldsymbol{\epsilon}$, and let $g(.) = \text{location} + \text{scale} \cdot \boldsymbol{\epsilon}$. 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.

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 is implemented with the following form:

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

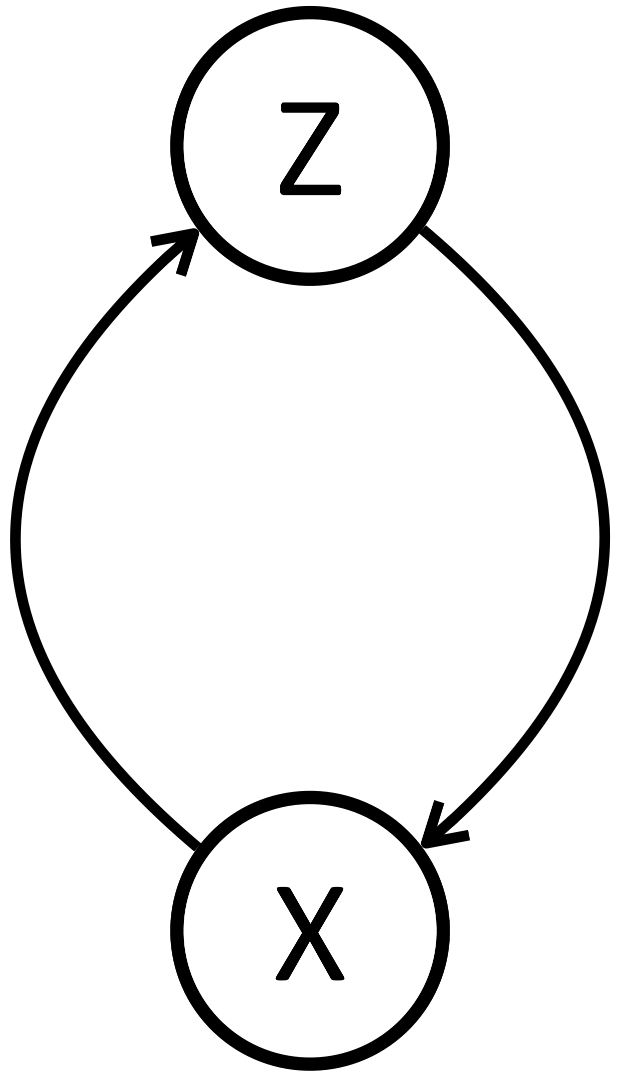
Autoencoder

ELBO

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

Autoencoder Loss

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



This is why it is called variational "autoencoder"

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

$$\int q_{\boldsymbol{\theta}}(\mathbf{z}) \log q_{\boldsymbol{\theta}}(\mathbf{z})\, d\mathbf{z} = \int \mathcal{N}(\mathbf{z}; \boldsymbol{\mu}, \boldsymbol{\sigma}^2) \log \mathcal{N}(\mathbf{z}; \boldsymbol{\mu}, \boldsymbol{\sigma}^2)\, d\mathbf{z}$$
$$= -\frac{J}{2}\log(2\pi) - \frac{1}{2}\sum_{j=1}^{J}(1 + \log \sigma_j^2)$$

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

Training VAEs

E-Step:

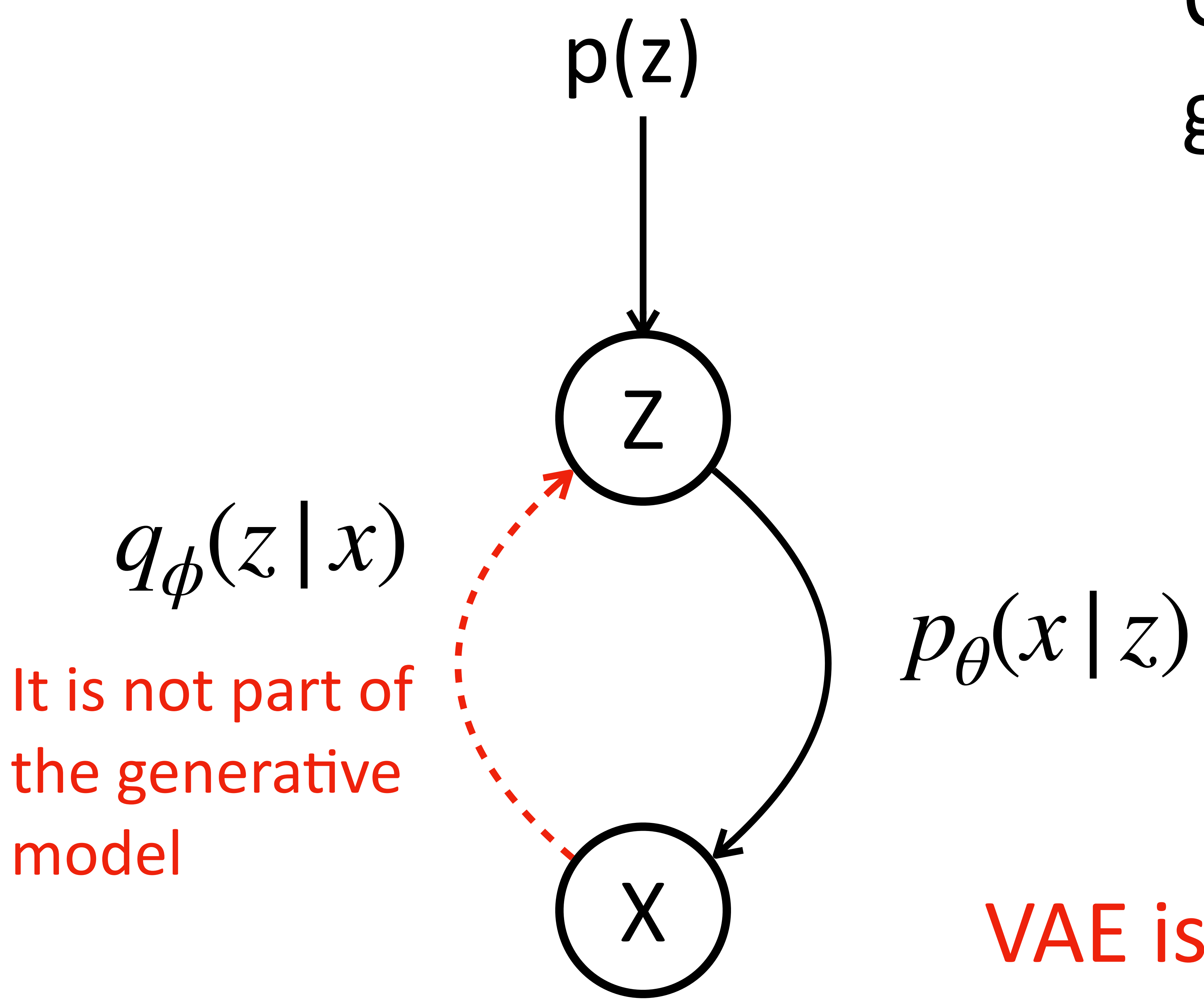
$$\text{argmax}_{\phi} \quad \underbrace{\mathbb{E}_{\mathbf{z}\sim q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})}[\log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})]}_{\text{Reconstruction Loss}} - \underbrace{D_{\mathrm{KL}}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})\|p(\mathbf{z}))}_{\text{KL Regularizer}}$$

M-Step:

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

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



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

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

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

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

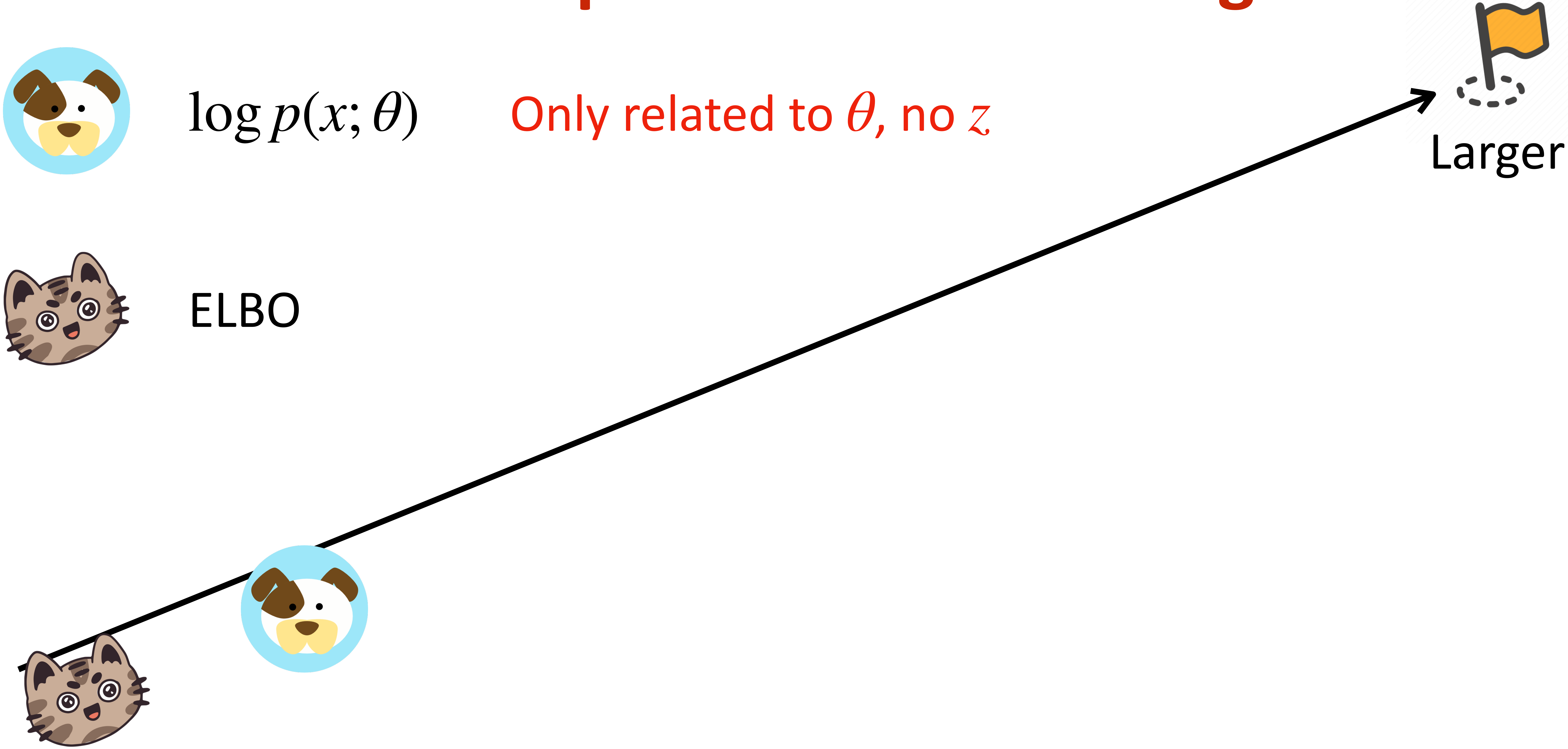
End-to-end, because the objectives are the same (ELBO)

VAE training is optimizing ELBO with gradient descent

Recap: EM is Hill Climbing

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

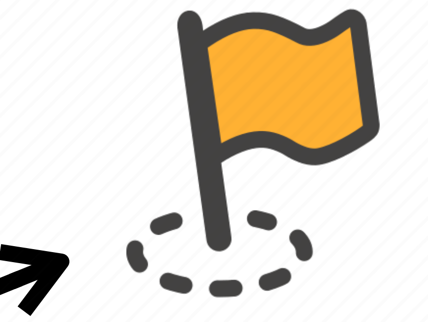
ELBO



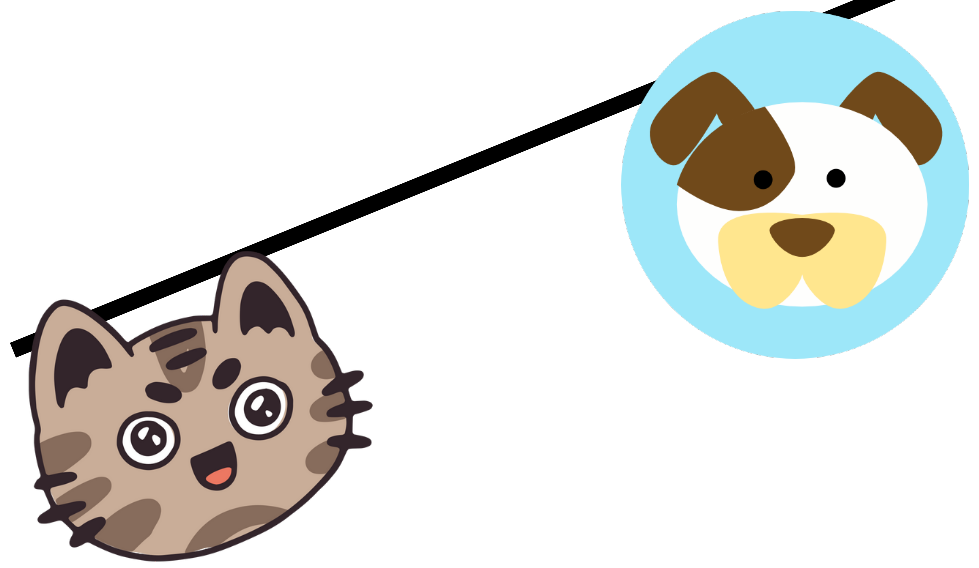
Recap: EM is Hill Climbing

$\log p(x;\theta)$

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

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

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

Is VAE training still Hill Climbing?

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

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

It just works in many cases

E-Step:

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

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

The Posterior Collapse Issue

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

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)

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

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

Reconstruction Loss - λ * KL regularizer

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:

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

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

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

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)

Published as a conference paper at ICLR 2019

LAGGING INFERENCE NETWORKS AND POSTERIOR COLLAPSE IN VARIATIONAL AUTOENCODERS

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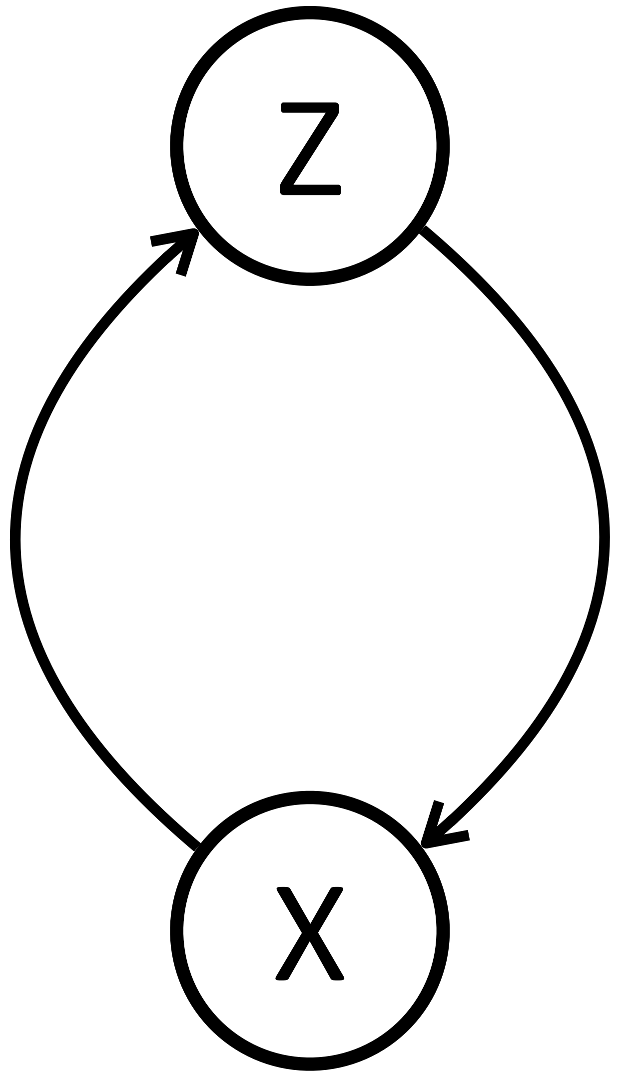
AutoEncoders

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

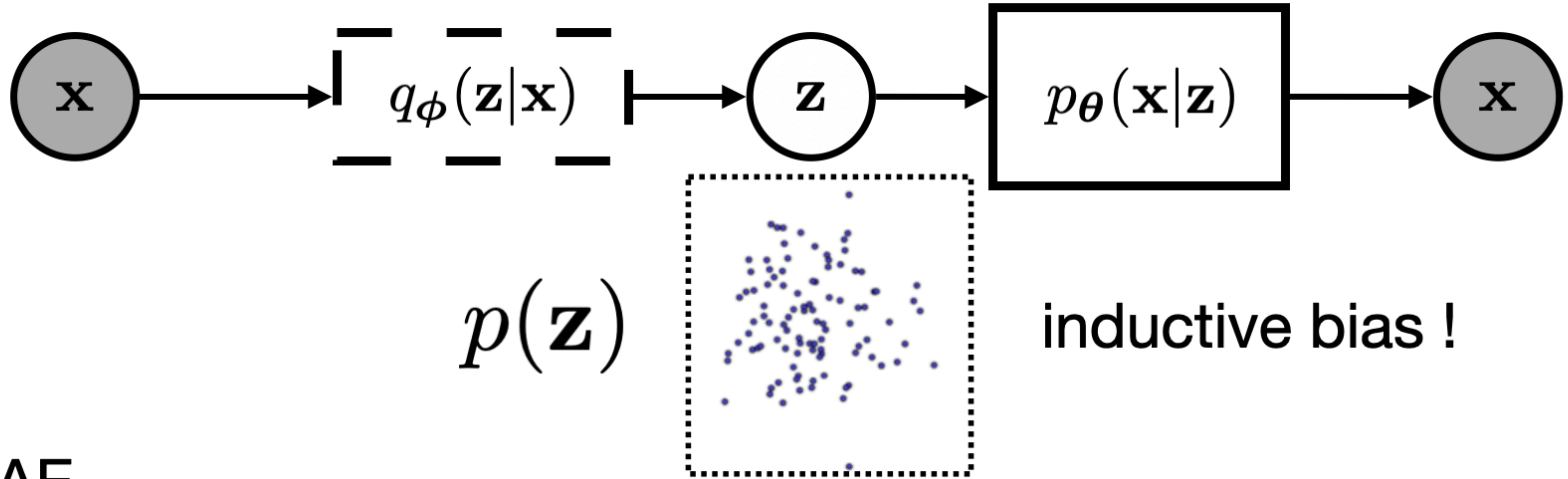
AE: $$\log p_\theta(x \,|\, q(x))$$



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?

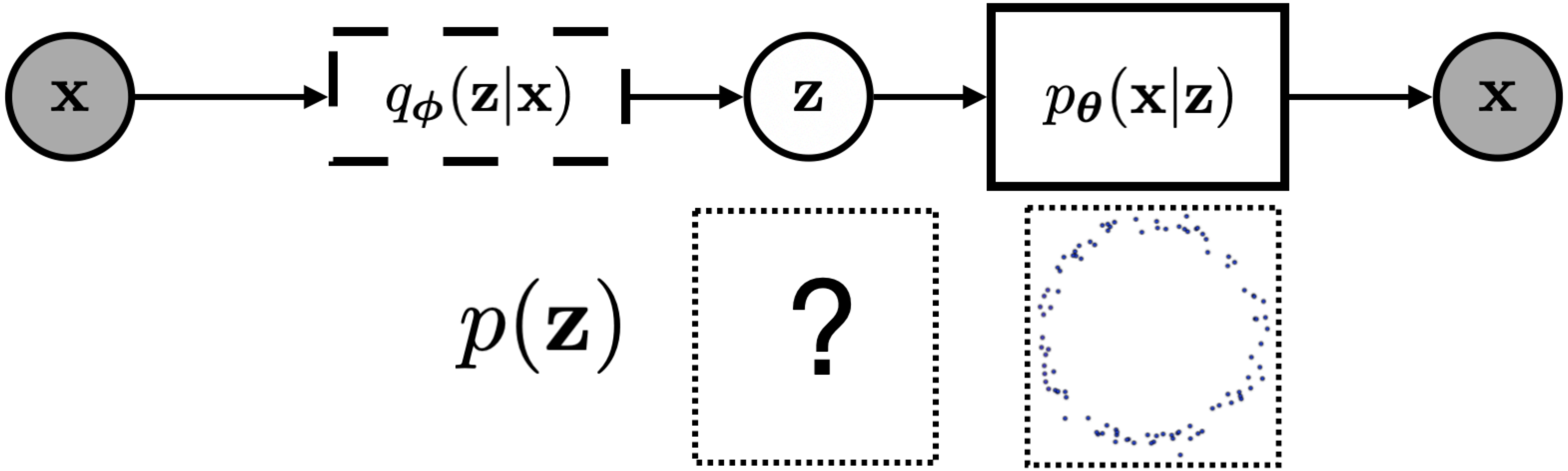
VAE v.s. AE

VAE



inductive bias !

AE



Generative Adversarial Nets

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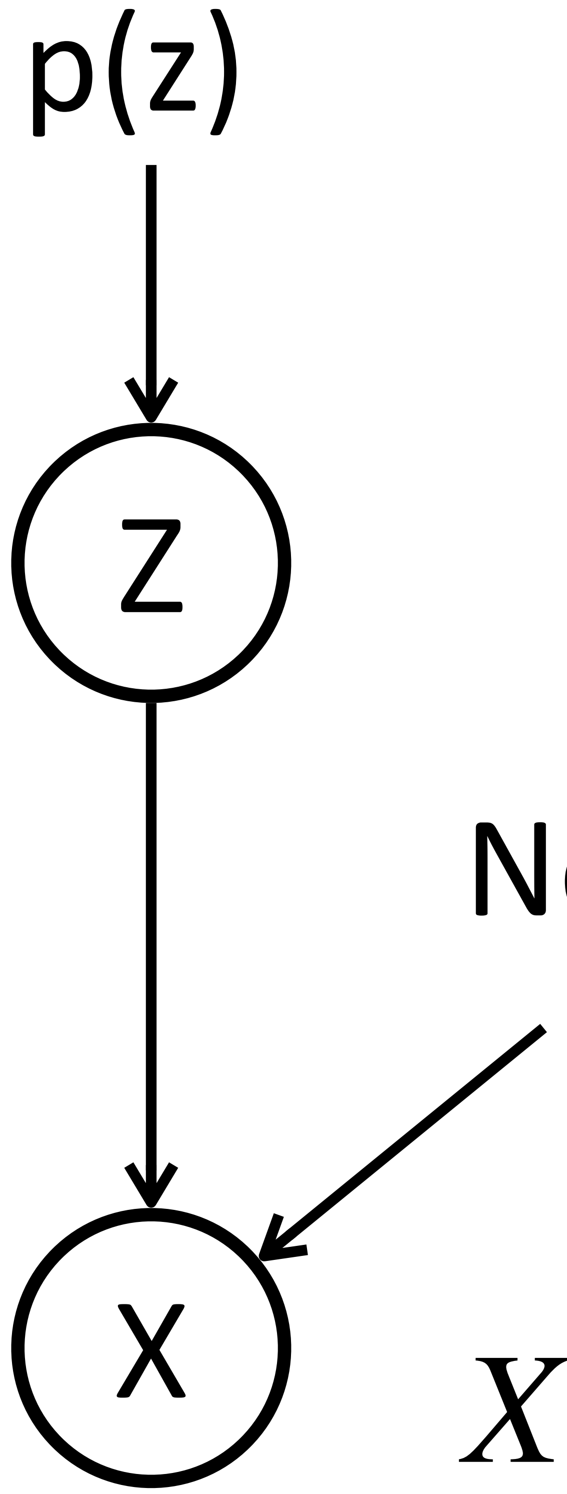
Generative Adversarial Networks

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

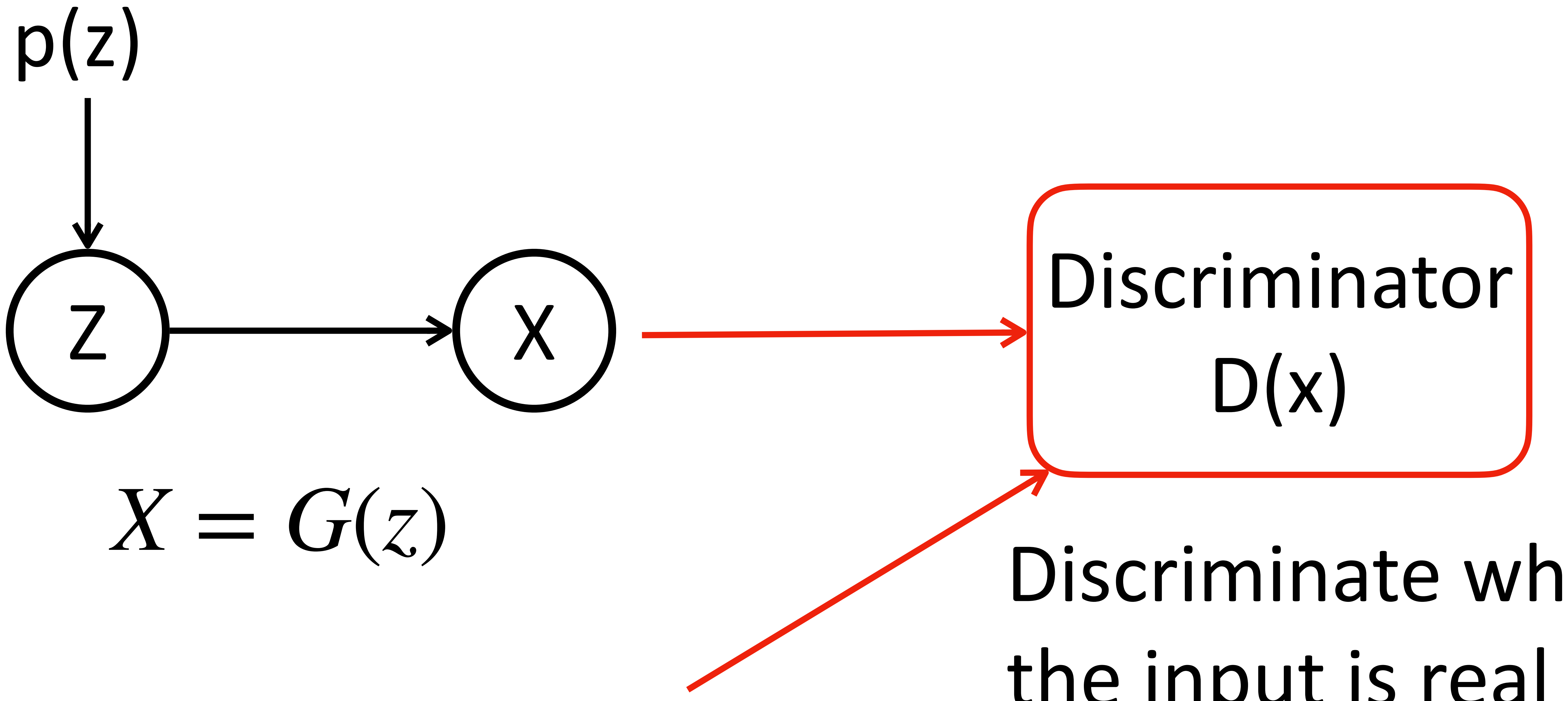
Can VAE use a deterministic x = G(z)?

Sometimes we call GANs *implicit* generative models

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

Training GANs

Computation Graph



$X = G(z)$

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

Discriminate whether the input is real or fake

1. Generator is trained to produce realistic examples to fool the discriminator
2. Discriminator is trained to discriminate real and fake examples

Training GANs

1. Generator is trained to produce realistic examples to fool the discriminator
2. Discriminator is trained to discriminate real and fake examples

The two objectives are against each other

Adversarial Game

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

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