CS769 Advanced NLP

Latent Variable Models

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Slides adapted from Graham

https://junjiehu.github.io/cs769-fall25/

Goal for Today

- **Variational Auto-encoder (VAE)**
  1. Maximize Evidence Lower Bound (ELBO)
  2. Reparamertizction trick
  3. Stabilizing Training
- **Discrete Latent Variable Models (LVM)**
  1. Enumerate
  2. Sampling
  3. Gumbel-softmax
- **LVM Applications in NLP**

Discriminative vs. Generative Models

- **Discriminative model:** calculate the probability of output given input P(Y|X)

- **Generative model:** calculate the probability of a variable P(X), or multiple variables P(X,Y)

- Which of the following models are discriminative vs. generative?

  - Standard BiLSTM POS tagger

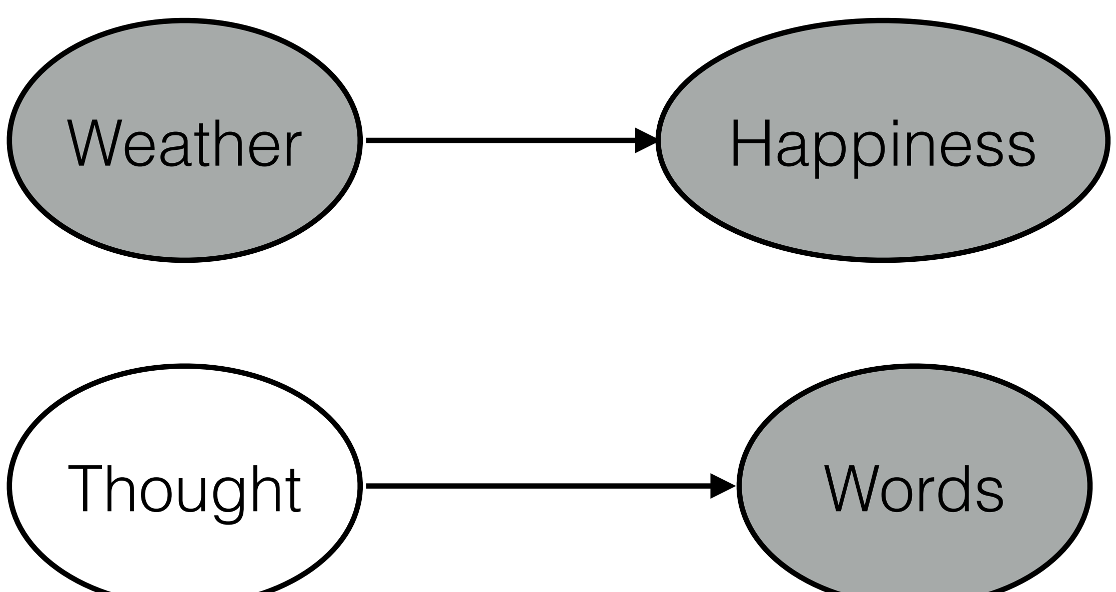
  - Language model

Types of Variables

- Random vs. deterministic variables:
  - **Random variable (R.V.):** is a math formalization of a object which depends on a random event. Namely, it defines a **function** that map an event to a numerical value. We usually use **uppercase letter *X, Y*** to denote R.V.. Once the event has been sampled, we get a real value of the R.V., we call this **realization of a R.V.**, and usually use **lowercase letter *x, y*** to denote them.
  - **Deterministic variable:** a variable that does not depend on any random event. We typically use ***a, b, c*** to denote them.
- Example:
  - X denotes a R.V. of the weather, X can be realized by taking values from a set (domain) {“rainy”, “sunny”, “cloudy”, ….}
  - P(X = “rainy”) provides a probability of a realization of the R.V. (i.e., a particular event)

Types of Variables

- Observed vs. Latent:
  - **Observed:** something that we can observe and measure from our data, e.g. X or Y
  - **Latent:** a variable that we assume exists, but we aren't given the value, namely something we don't have data for
- In graphical models, observed variables are typically shaded nodes, and latent variables are typically unshaded nodes.



Marginal over latent variables is usually intractable (not computable in a reason time).

$$p(w) = \int_T p(T, w) dT$$

Latent Variable Models

- A vector of latent variables $\mathbf{z}$ in a high-dim space $\mathcal{Z}$ which we can sample from some PDF $p(\mathbf{z})$ over $\mathcal{Z}$
- For every observed $\mathbf{x}$ in our dataset, there is a $\mathbf{z}$ that causes the model to generate $\mathbf{x}$
- A latent variable model (LVM) is a probability distribution over two sets of variables $\mathbf{x}$, $\mathbf{z}$:

$$p(\mathbf{x}|\mathbf{z};\theta)$$

Maximum Likelihood Framework

- Maximize the probability of each x in the training set under the generative process according to:

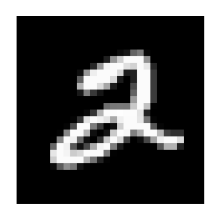
$$p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{z};\theta)p(\mathbf{z})d\mathbf{z}$$

Why LVM?

- Intuitively, latent variable **z** enables the model to first decide which property to generate before it assigns values to the output **x**

- Example:

  - Sample a LV z from the set [0,…9] before generating an image for the digit

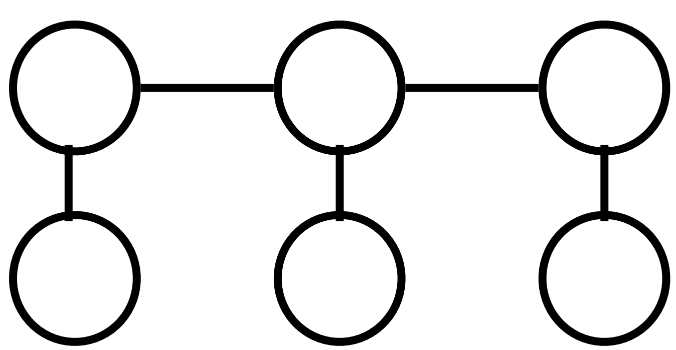
    z=2 -> x= 

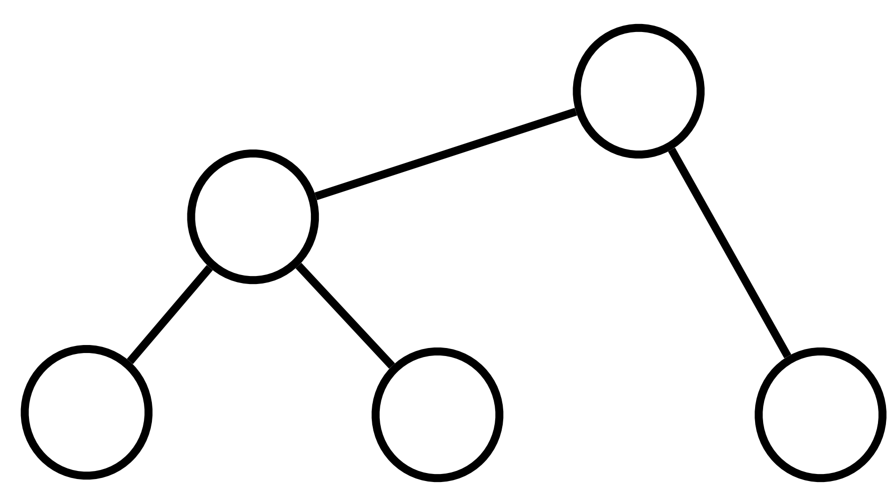
  - Sample a sentiment from {positive, negative} before generating a positive/negative movie review.

    z="negative" -> x= "This is a bad movie."

What Types of Latent Variables?

- Latent continuous vector (e.g. variational auto-encoder)
- Latent discrete vector (e.g. topic model)
- Latent structure (e.g. HMM or tree-structured model)



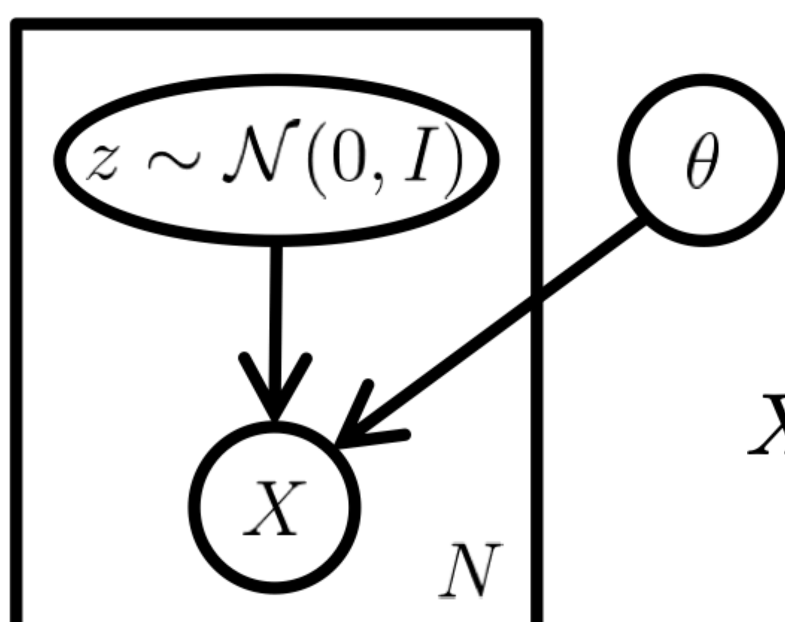


Variational Auto-encoders

(Kingma and Welling 2014)

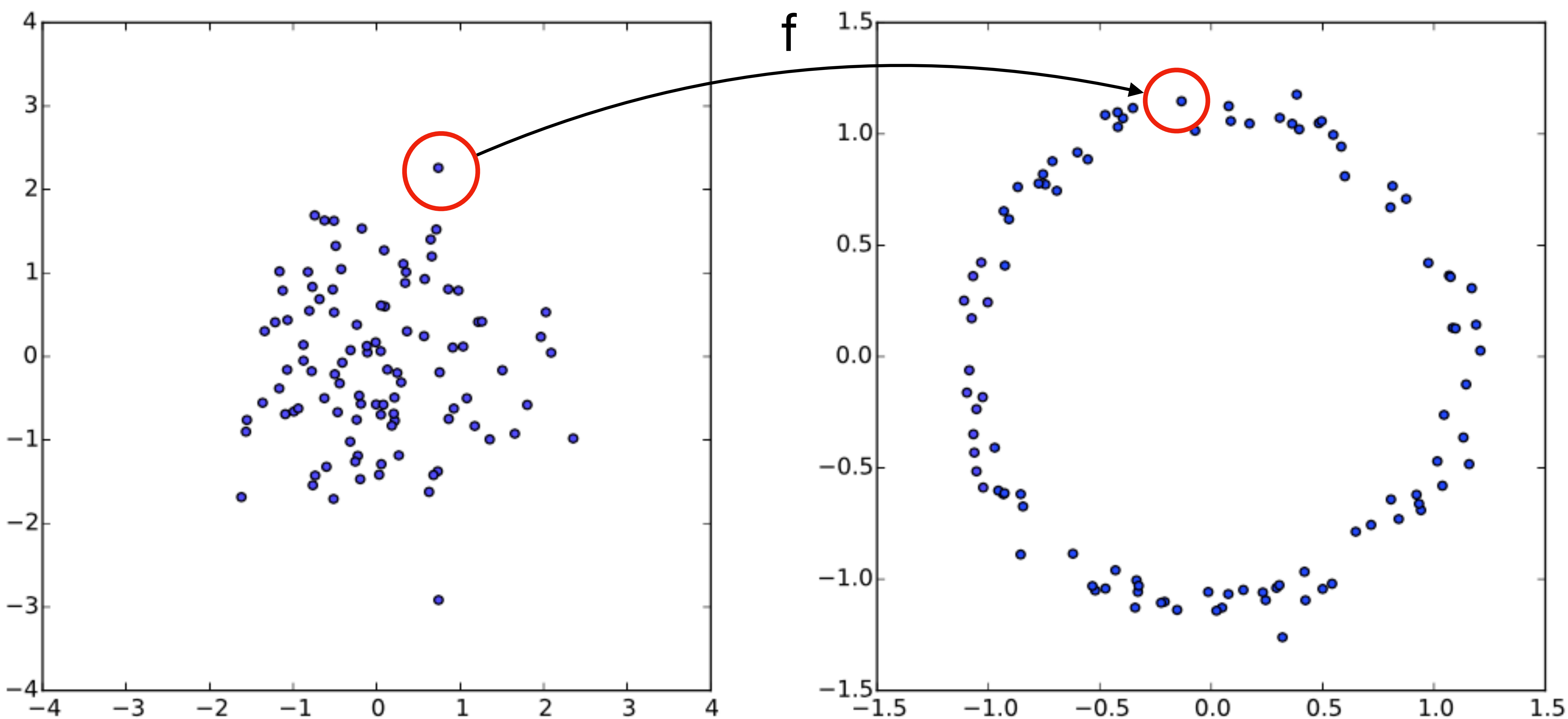
VAE as a Graphical Model

- We have a random variable ***X*** for our dataset
- We have a latent variable **z** sampled from a Gaussian
- We have a deterministic function $f(\mathbf{z};\theta)$ that maps $\mathbf{z}$ to the data space $\mathcal{X}$. If $\mathbf{z}$ is a random variable (r.v.) in $\mathcal{Z}$, then $f(\mathbf{z};\theta)$ is also a r.v. in $\mathcal{X}$
- If we repeat this sampling *N* times, we hope to approximate X by $f(\mathbf{z};\theta)$



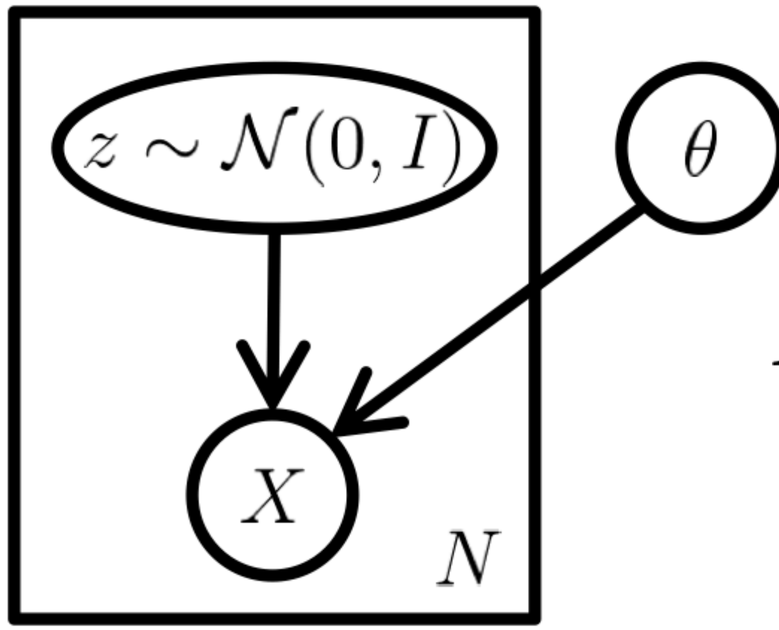
$$X \approx \frac{1}{N} \sum_{z\sim\mathcal{N}(0,I)} f(\mathbf{z};\theta)$$

An Example (Goersch 2016)



$\mathbf{z}$ $\quad\quad$ $\mathbf{x} = f(\mathbf{z}) = \mathbf{z}/10 + \mathbf{z}/\|\mathbf{z}\|$ $\quad\quad$ $\mathbf{x}$

A probabilistic perspective on Variational Auto-Encoder



$$X \approx \frac{1}{N} \sum_{z \sim \mathcal{N}(0,I)} f(\mathbf{z}; \theta)$$

- For each datapoint i :
    - Draw latent variables $z_i \sim p(z)$ (prior)
    - Draw data point $x_i \sim p_\theta(x|z)$
- Joint probability distribution over data and latent variables:

$$p(x, z) = p(z) p_\theta(x|z)$$

- Similar to Naive Bayes, HMM: only the prior differs

What is Our Loss Function?

- We would like to maximize the corpus log likelihood

$$\log P(\mathcal{X}) = \sum_{\boldsymbol{x} \in \mathcal{X}} \log P(\boldsymbol{x}; \theta)$$

- For a single example, the marginal likelihood is

$$P(\boldsymbol{x}; \theta) = \int P(\boldsymbol{x} \mid \boldsymbol{z}; \theta) P(\boldsymbol{z}) d\boldsymbol{z}$$

- We can approximate this by sampling **z**s then summing

$$P(\boldsymbol{x}; \theta) \approx \sum_{\boldsymbol{z} \in S(\boldsymbol{x})} P(\boldsymbol{x} | \boldsymbol{z}; \theta) \quad \text{where} \quad S(\boldsymbol{x}) := \{\boldsymbol{z}'; \boldsymbol{z}' \sim P(\boldsymbol{z})\}$$

Variational Inference

Two tasks of interest:

- Learn the parameters θ of $p_\theta(x|z)$
- **Inference** over z with the *posterior* distribution: $p_\theta(z|x)$ given input x, what are its latent factors?

$$p_\theta(z|x) = \frac{p_\theta(x|z)p(z)}{p(x)}$$

$$p(x) = \int p(z)p_\theta(x|z)dz$$ <- intractable

- However, as $p(x)$ is intractable $p_\theta(z|x)$ is also intractable.
- Solution: **Variational inference** approximates the posterior $p_\theta(z|x)$ with a family of distributions $q_\phi(z|x)$

Variational Inference

- Variational inference approximates the true posterior $p_\theta(z|x)$ with a family of distributions $q_\phi(z|x)$

$$\text{minimize}: \ \mathrm{KL}(q_\phi(z|x)||p_\theta(z|x))$$

- One other target is to maximize the log-data likelihood which can be rewritten as:

$$\log p(x) = \mathrm{ELBO} + \mathrm{KL}(q_\phi(z|x)||p_\theta(z|x))$$

- Combining the above two, this is equivalent to maximize the **Evidence Lower Bound (ELBO)**

$$\mathrm{ELBO} = \mathbb{E}_{q_\phi(z|x)}[\log p_\theta(x|z)] - \mathrm{KL}(q_\phi(z|x)||p(z))$$

$$\mathrm{KL}(q||p) \geq 0 => \log p(x) \geq \mathrm{ELBO}$$

Variational Inference

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- **Evidence Lower Bound (ELBO)**

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Variational Inference

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$$\text{minimize}: \ \mathrm{KL}(q_\phi(z|x)||p_\theta(z|x))$$

$$\text{maximize}: \log p(x) = \mathrm{ELBO} + \mathrm{KL}(q_\phi(z|x)||p_\theta(z|x))$$

$$\quad\quad\quad\quad\quad \uparrow \quad\quad\quad\quad \uparrow \quad\quad\quad\quad\quad\quad\quad \downarrow$$

- Combining the above two objectives, it is equivalent to maximize ELBO

$$\text{maximize}: \mathrm{ELBO}$$

Variational Auto-Encoders

$$\log p_{\boldsymbol{\theta}}(\mathbf{x}) \geq \mathrm{ELBO}$$

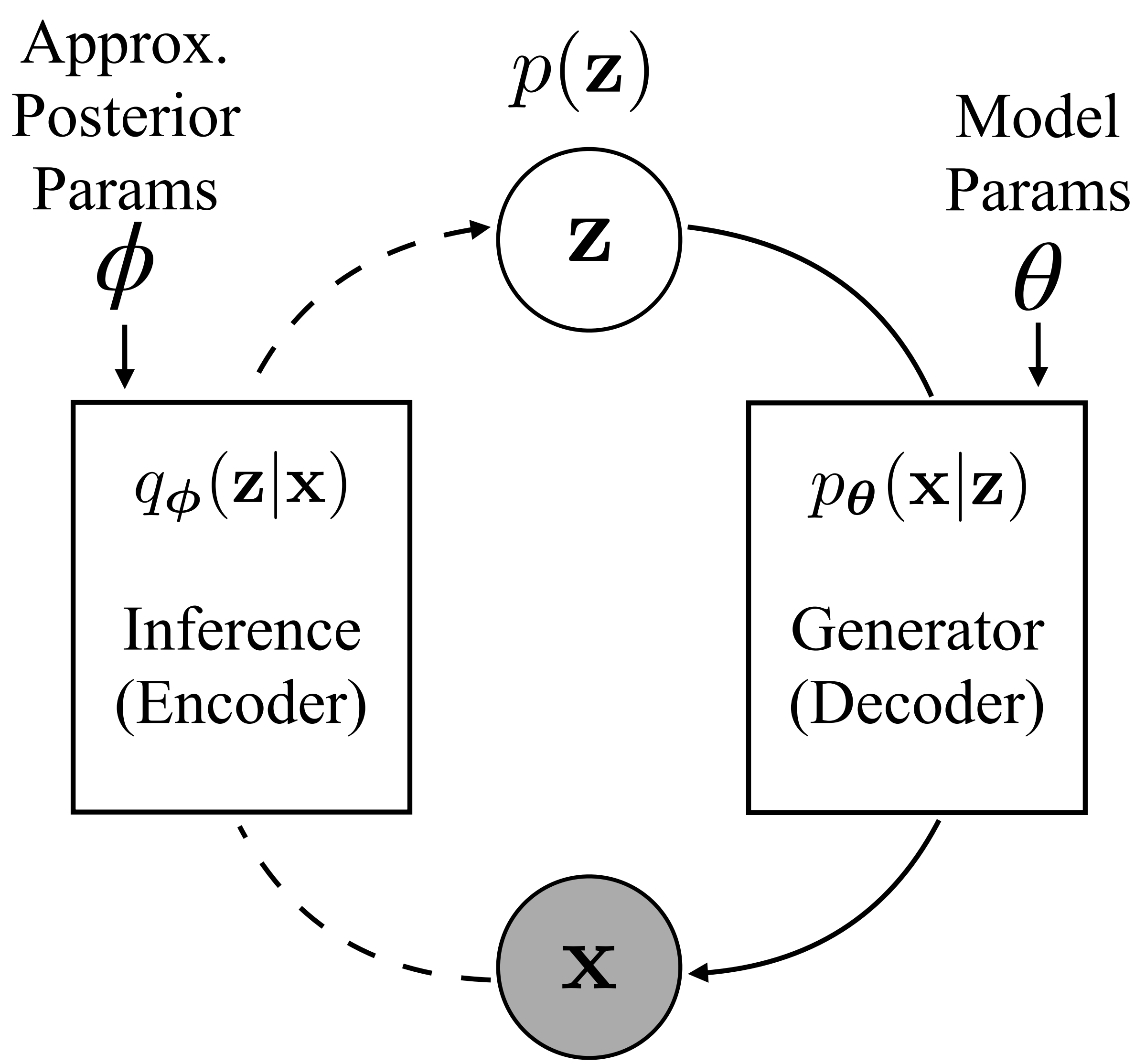
$$\underbrace{\mathbb{E}_{\mathbf{z}\sim q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})}[\log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})]}_{\text{Reconstruction Loss}} - \underbrace{D_{\mathrm{KL}}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})\|p(\mathbf{z}))}_{\text{KL Regularizer}}$$

The inequality holds for any $q_\phi(z|x)$, but the lower bound is tight only if $p_\theta(z|x) = q_\phi(z|x)$

$p_\theta(z|x)$ is intractable

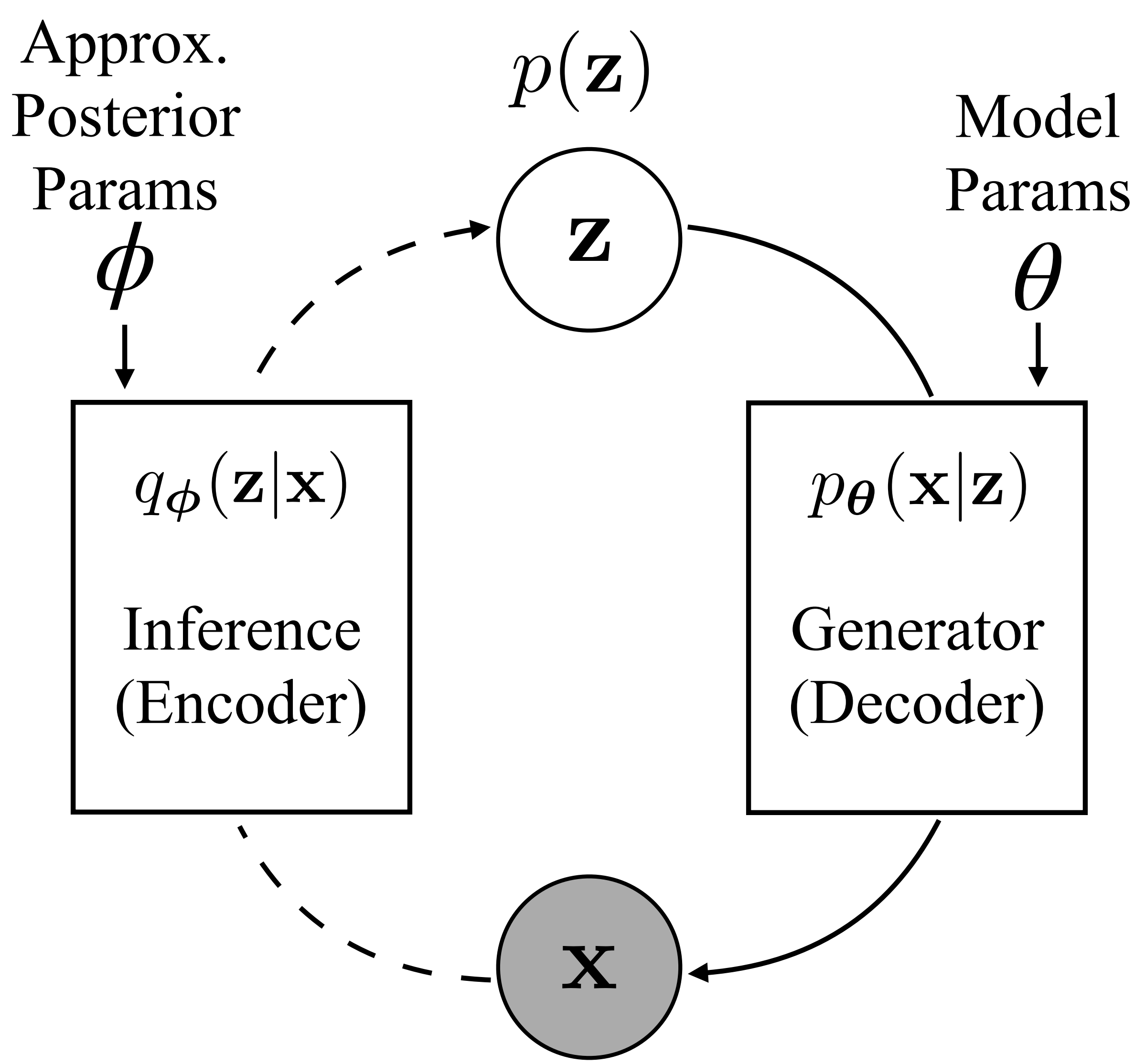
Variational Autoencoders

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



Variational Autoencoders

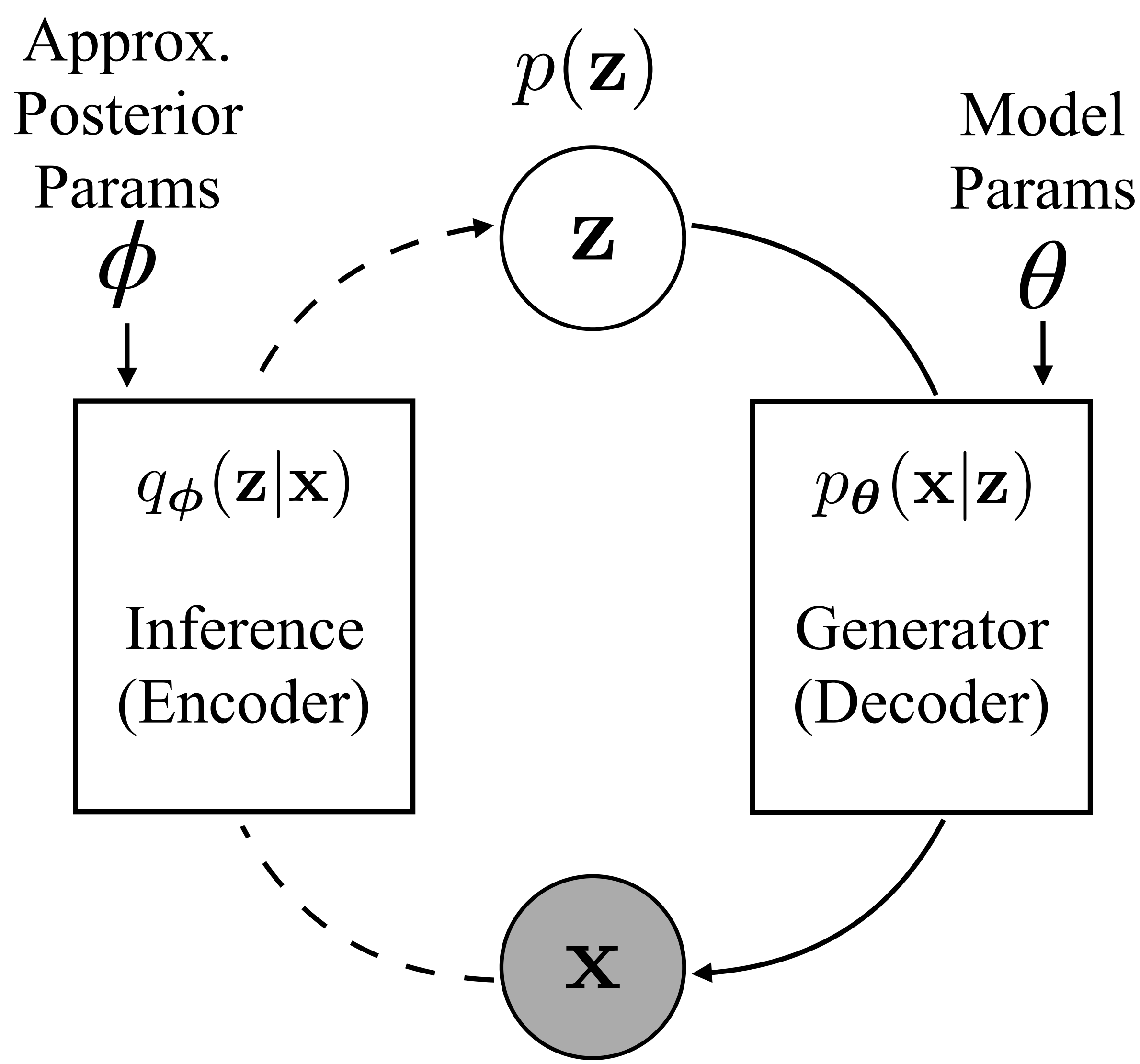
$$\log p_{\boldsymbol{\theta}}(\mathbf{x}) >= \underbrace{\mathbb{E}_{\mathbf{z}\sim q_{\phi}(\mathbf{z}|\mathbf{x})}[\log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})]}_{\text{Reconstruction Loss}} - \underbrace{D_{\mathrm{KL}}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})\|p(\mathbf{z}))}_{\text{KL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



Regularized Autoencoder

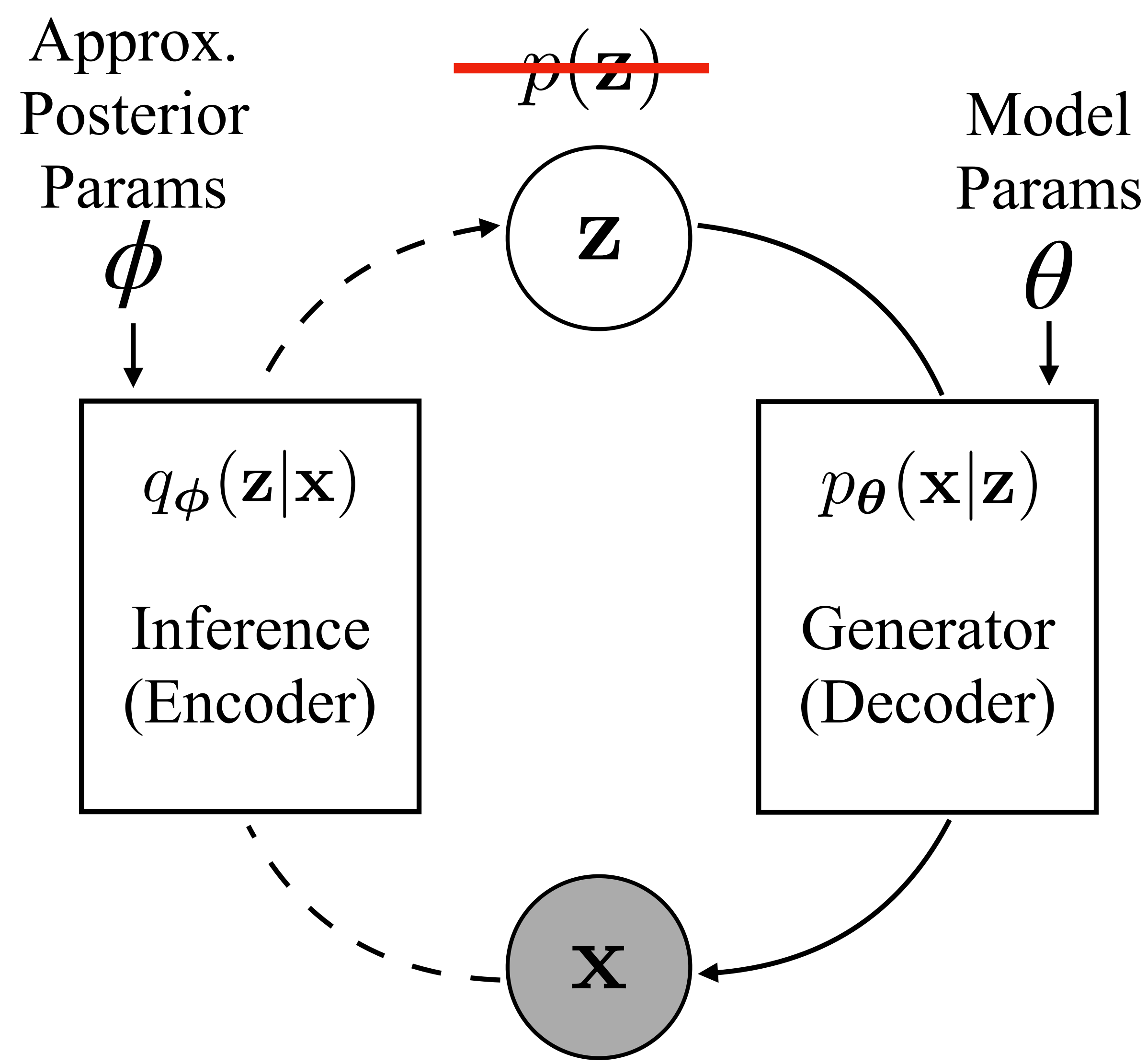
Why prior ?

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



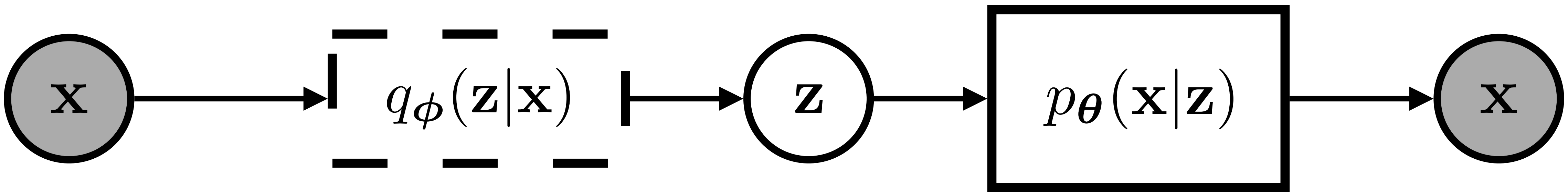
Why prior ?

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



VAE vs. AE

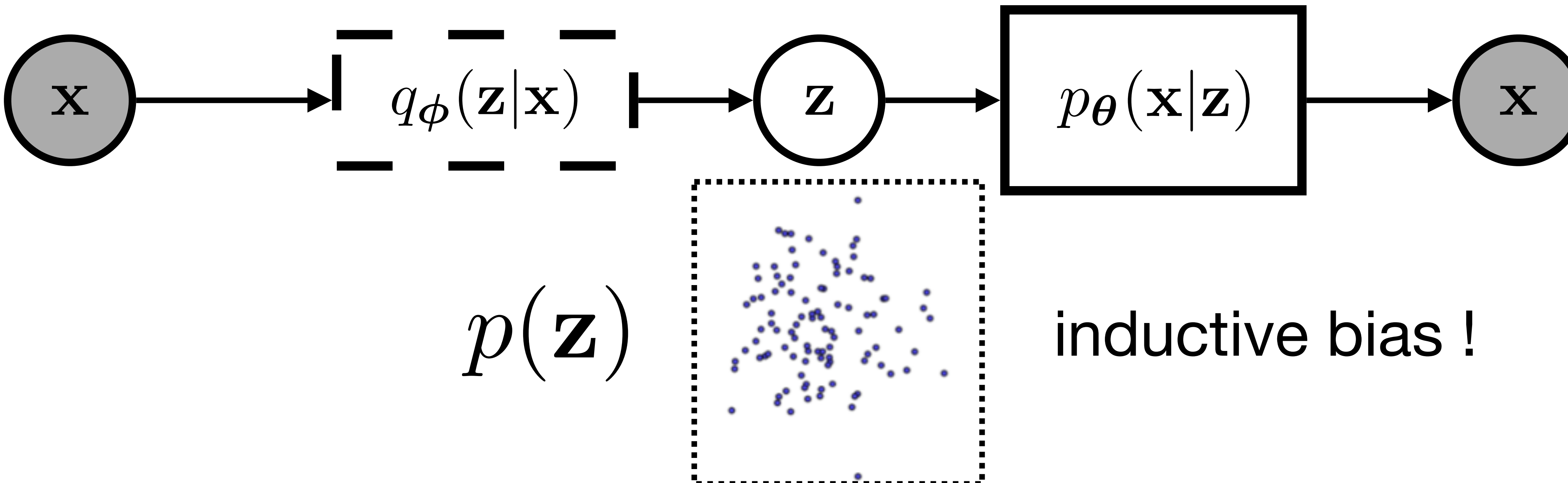
VAE



$\mathbf{x}$
$q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$
$\mathbf{z}$
$p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})$
$\mathbf{x}$

VAE vs. AE

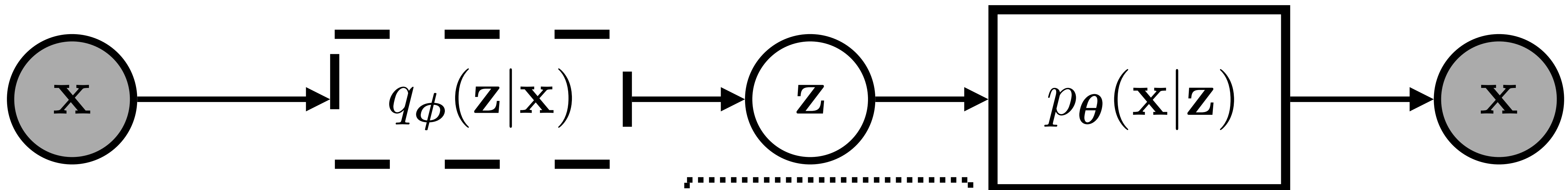
VAE



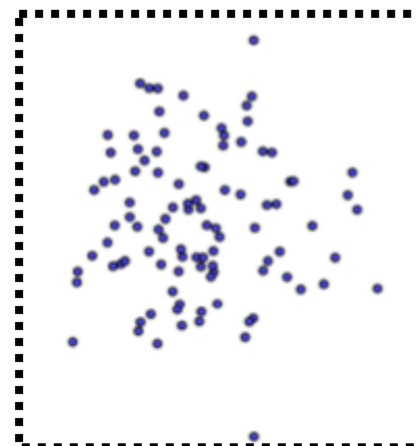
inductive bias !

VAE vs. AE

VAE

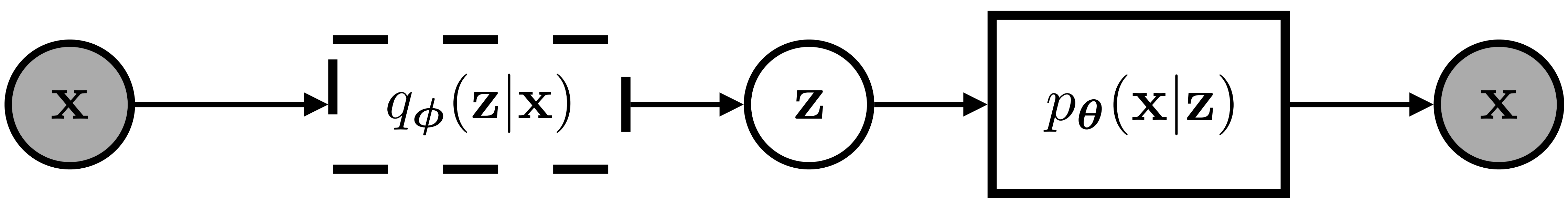


$p(\mathbf{z})$

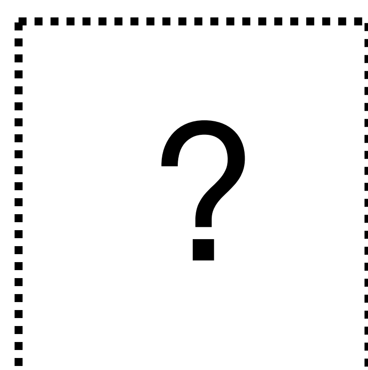


inductive bias !

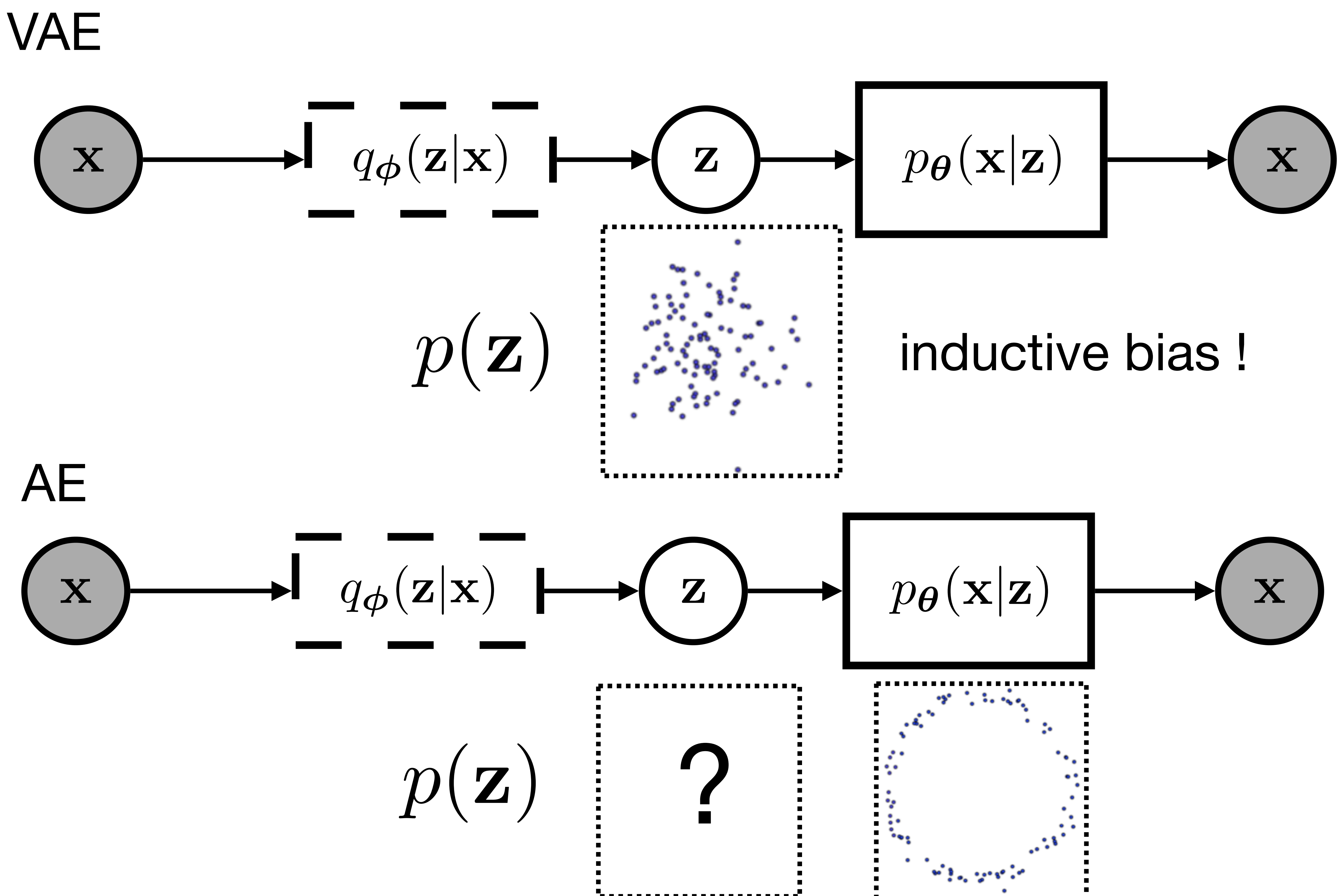
AE



$p(\mathbf{z})$



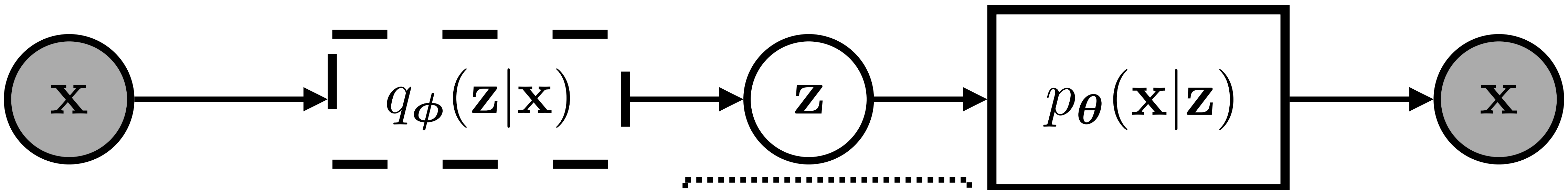
VAE vs. AE



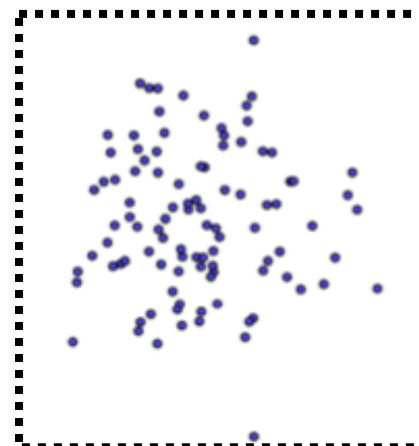
VAE
$\mathbf{x}$
$q_{\phi}(\mathbf{z}|\mathbf{x})$
$\mathbf{z}$
$p_{\theta}(\mathbf{x}|\mathbf{z})$
$\mathbf{x}$
$p(\mathbf{z})$
inductive bias !
AE
$\mathbf{x}$
$q_{\phi}(\mathbf{z}|\mathbf{x})$
$\mathbf{z}$
$p_{\theta}(\mathbf{x}|\mathbf{z})$
$\mathbf{x}$
$p(\mathbf{z})$
?

VAE vs. AE

VAE

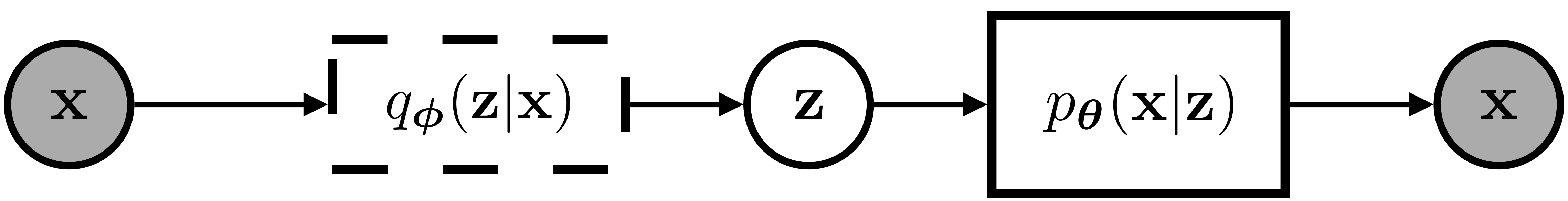


$p(\mathbf{z})$



inductive bias !

AE

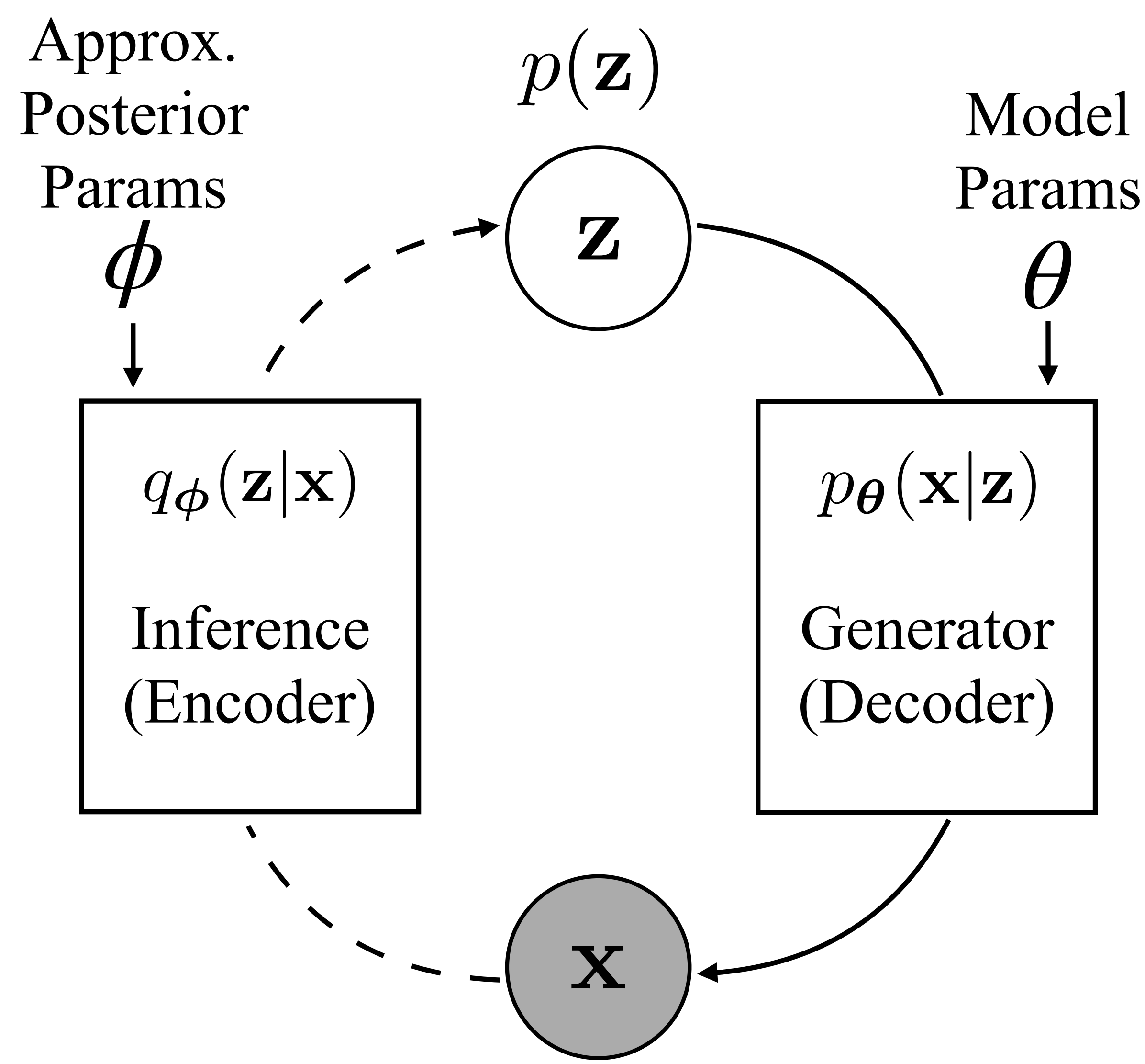


AE is not generative model:

(1) Can’t sample new data from AE
(2) Can’t compute the log likelihood of data x

Training of VAE

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



Problem!
Sampling Breaks Backprop

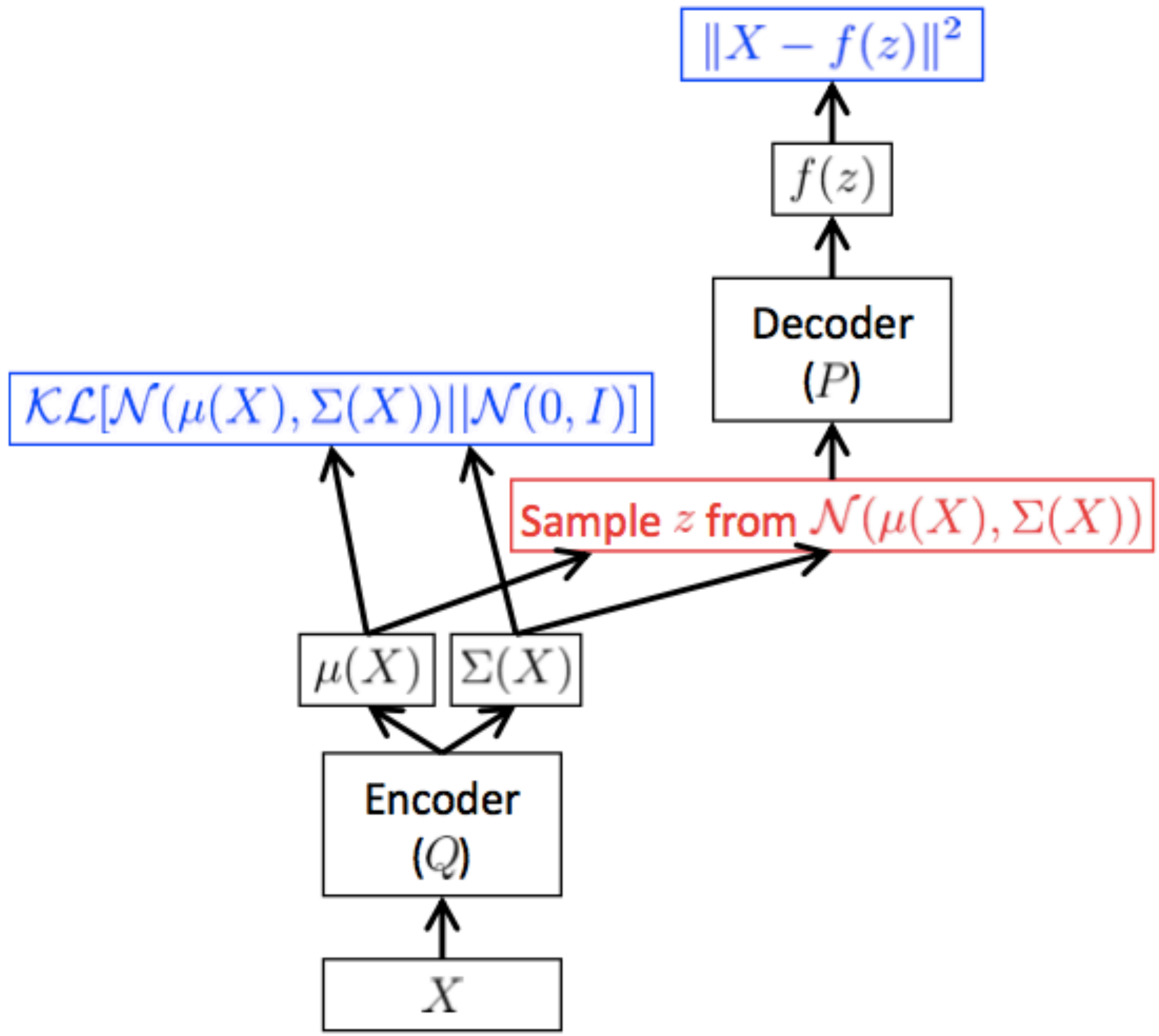


Figure Credit: Doersch (2016)

Solution:
Re-parameterization Trick

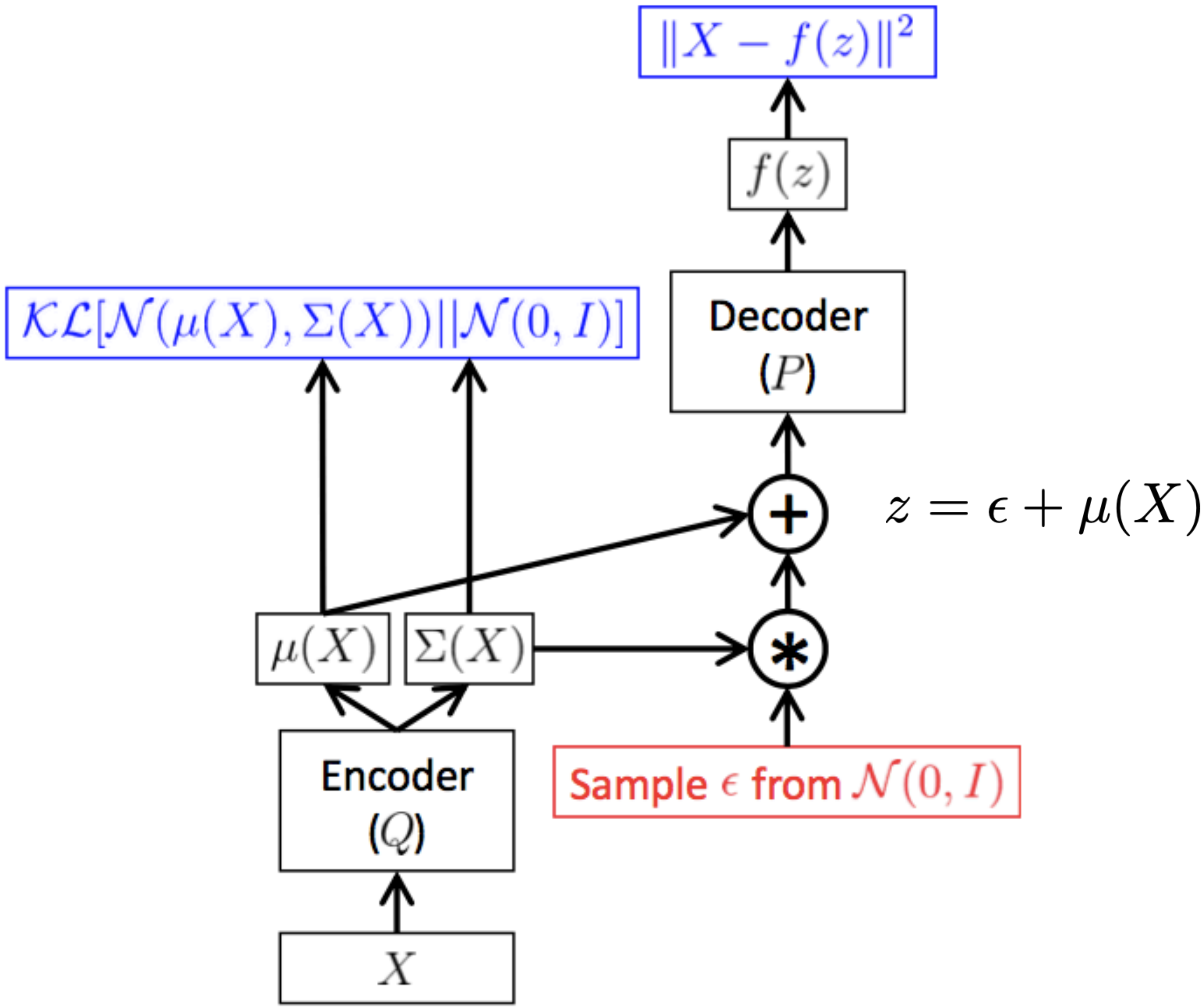


Figure Credit: Doersch (2016)

An Example: Generating Sentences w/ Variational Autoencoders

Generating from Language Models

- **Remember:** using ancestral sampling, we can generate from a normal language model

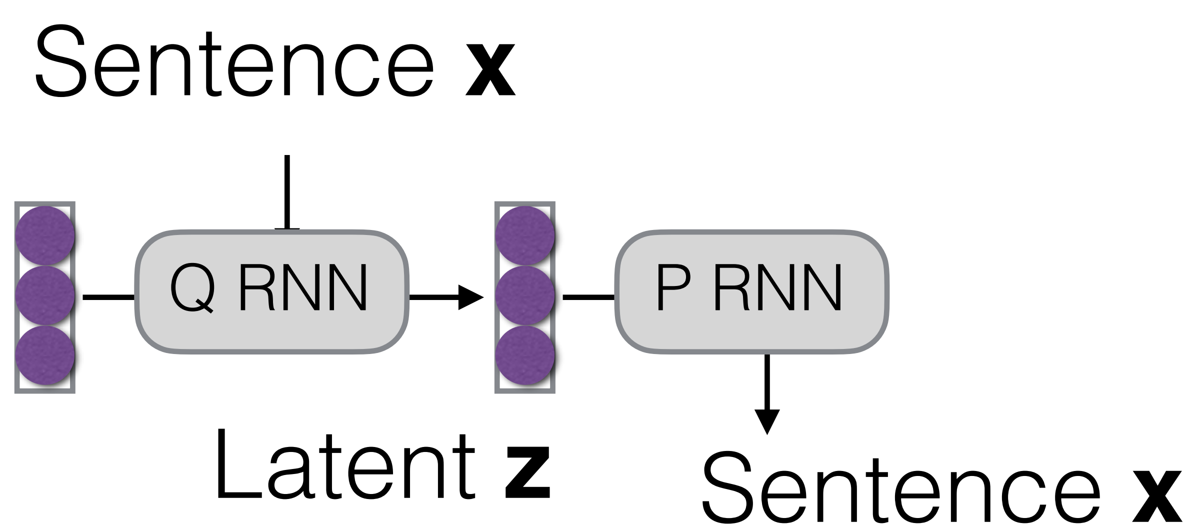
while x_{j-1} != “</s>”:
$\quad x_j \sim P(x_j \mid x_1, \ldots, x_{j-1})$

- We can also generate conditioned on something P(**y**|**x**) (e.g. translation, image captioning)

while y_{j-1} != “</s>”:
$\quad y_j \sim P(y_j \mid X, y_1, \ldots, y_{j-1})$

Generating Sentences from a Continuous Space (Bowman et al. 2015)

- The VAE-based approach is conditional language model that conditions on a latent variable **z**
- Like an encoder-decoder, but latent representation is latent variable, input and output are identical



Motivation for Latent Variables

- Allows for a **consistent latent space** of sentences?
  - e.g. interpolation between two sentences

Standard encoder-decoder

i went to the store to buy some groceries .
i store to buy some groceries .
i were to buy any groceries .
horses are to buy any groceries .
horses are to buy any animal .
horses the favorite any animal .
horses the favorite favorite animal .
horses are my favorite animal .

VAE

" i want to talk to you . "
"i want to be with you . "
"i do n't want to be with you . "
i do n't want to be with you .
she did n't want to be with him .

he was silent for a long moment .
he was silent for a moment .
it was quiet for a moment .
it was dark and cold .
there was a pause .
it was my turn .

- **More robust to noise?** VAE can be viewed as standard model + regularization.

Difficulties in Training

- Of the two components in the VAE objective, the KL divergence term is much easier to learn!

$$\underbrace{\mathbb{E}_{\boldsymbol{z}\sim Q(\boldsymbol{z}|\boldsymbol{x})}[\log P(\boldsymbol{x} \mid \boldsymbol{z})]}_{\text{Requires good generative model}} - \underbrace{\mathcal{KL}[Q(\boldsymbol{z} \mid \boldsymbol{x})||P(\boldsymbol{z})]}_{\text{Just need to set the mean/variance of Q to be same as P}}$$

- Results in the model learning to rely solely on decoder and ignore latent variable ($P(x|z) = P(x)$) -> **Posterior Collapse**

Solution 1:
KL Divergence Annealing

- Basic idea: Multiply KL term by a constant λ starting at zero, then gradually increase to 1
- Result: model can learn to use **z** before getting penalized

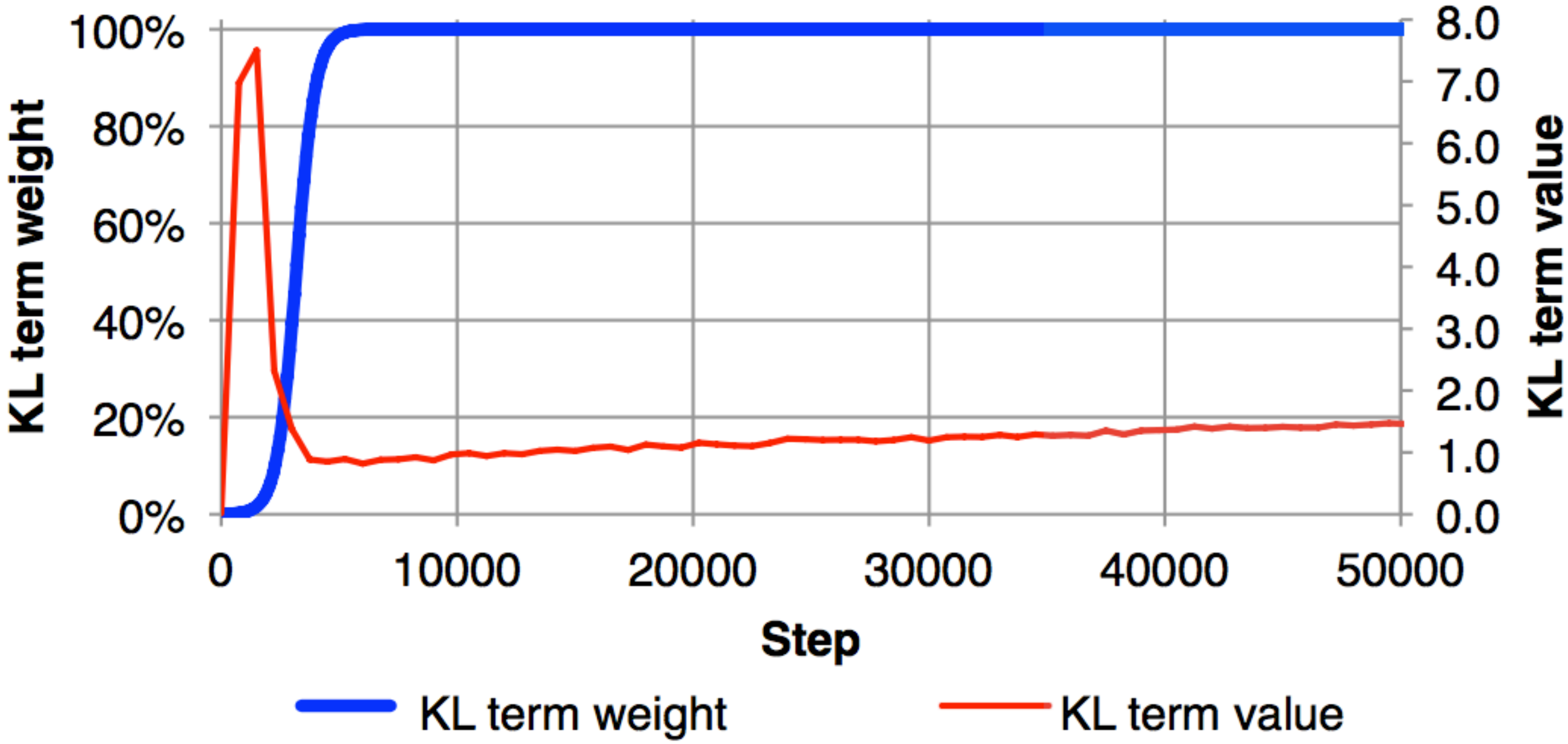


Figure Credit: Bowman et al. (2017)

Solution 2: Free bits / KL thresholding

- Free bits replaces the KL term in ELBO with a hinge loss that maximize each component of the original KL with a constant:

$$\sum_i \max[\lambda, D_{\mathrm{KL}}(q_\phi(z_i|x)||p(z_i))]$$

- λ :Target rate

Solution 3: Weaken the Decoder

- But theoretically still problematic: it can be shown that the optimal strategy is to ignore **z** when it is not necessary (Chen et al. 2017)
- Solution: weaken decoder P(**x**|**z**) so using **z** is essential
  - Use word dropout to occasionally skip inputting previous word in **x** (Bowman et al. 2015)
  - Use a convolutional decoder w/ limited context (Yang et al. 2017)

Solution 4:
Aggressive Inference Network Learning

$$\max_{\boldsymbol{\theta},\boldsymbol{\phi}} \quad \underbrace{\log p_{\boldsymbol{\theta}}(\mathbf{x})}_{\text{marginal log data likelihood}} \quad - \quad \underbrace{D_{\mathrm{KL}}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})|p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x}))}_{\text{agreement between approximate and model posteriors}}$$

$$\downarrow$$

$$\max_{\boldsymbol{\theta}} \max_{\boldsymbol{\phi}} \quad \underbrace{\log p_{\boldsymbol{\theta}}(\mathbf{x})}_{\text{marginal log data likelihood}} \quad - \quad \underbrace{D_{\mathrm{KL}}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})|p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x}))}_{\text{agreement between approximate and model posteriors}}$$

(He et al. 2019)

Handling Discrete Latent Variables

Discrete Latent Variables?

- Many variables are better treated as discrete
  - Part-of-speech of a word
  - Class of a question
  - Writer traits (left-handed or right-handed, etc.)
- How do we handle these?

Method 1: Enumeration

- For discrete variables, our integral is a sum

$$P(\boldsymbol{x};\theta) = \sum_{\boldsymbol{z}} P(\boldsymbol{x} \mid \boldsymbol{z};\theta)P(\boldsymbol{z})$$

- If the number of possible configurations for **z** is small, we can just sum over all of them

Method 2: Sampling

- Randomly sample a subset of configurations of **z** and optimize with respect to this subset

- Various flavors:
  - Minimum risk training
  - Maximize ELBO loss

- Score function gradient estimator - Policy Gradient Method
  - Unbiased estimator but high variance - need to control variance

Method 3: Reparameterization

(Maddison et al. 2017, Jang et al. 2017)

- Reparameterization also possible for discrete variables!

Original Categorical Sampling Method:

$$\hat{\boldsymbol{z}} = \text{cat-sample}(P(\boldsymbol{z} \mid \boldsymbol{x}))$$

Reparameterized Method

$$\hat{\boldsymbol{z}} = \text{argmax}(\log P(\boldsymbol{z} \mid \boldsymbol{x}) + \text{Gumbel(0,1)})$$

where the Gumbel distribution is

$$\text{Gumbel}(0, 1) = -\log(-\log(\text{Uniform(0,1)}))$$

- Backprop is still not possible, due to argmax

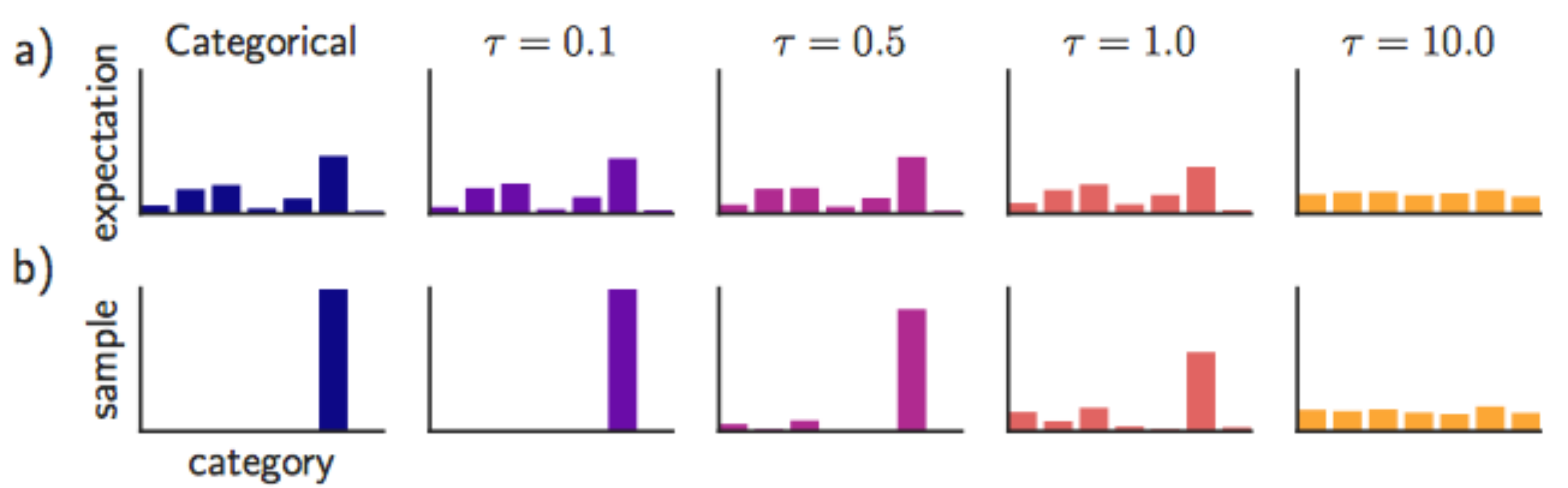
Gumbel-Softmax

- A way to soften the decision and allow for continuous gradients

- Instead of argmax, take softmax with temperature τ

$$\hat{\boldsymbol{z}} = \mathrm{softmax}((\log P(\boldsymbol{z} \mid \boldsymbol{x}) + \mathrm{Gumbel}(0{,}1))^{1/\tau})$$

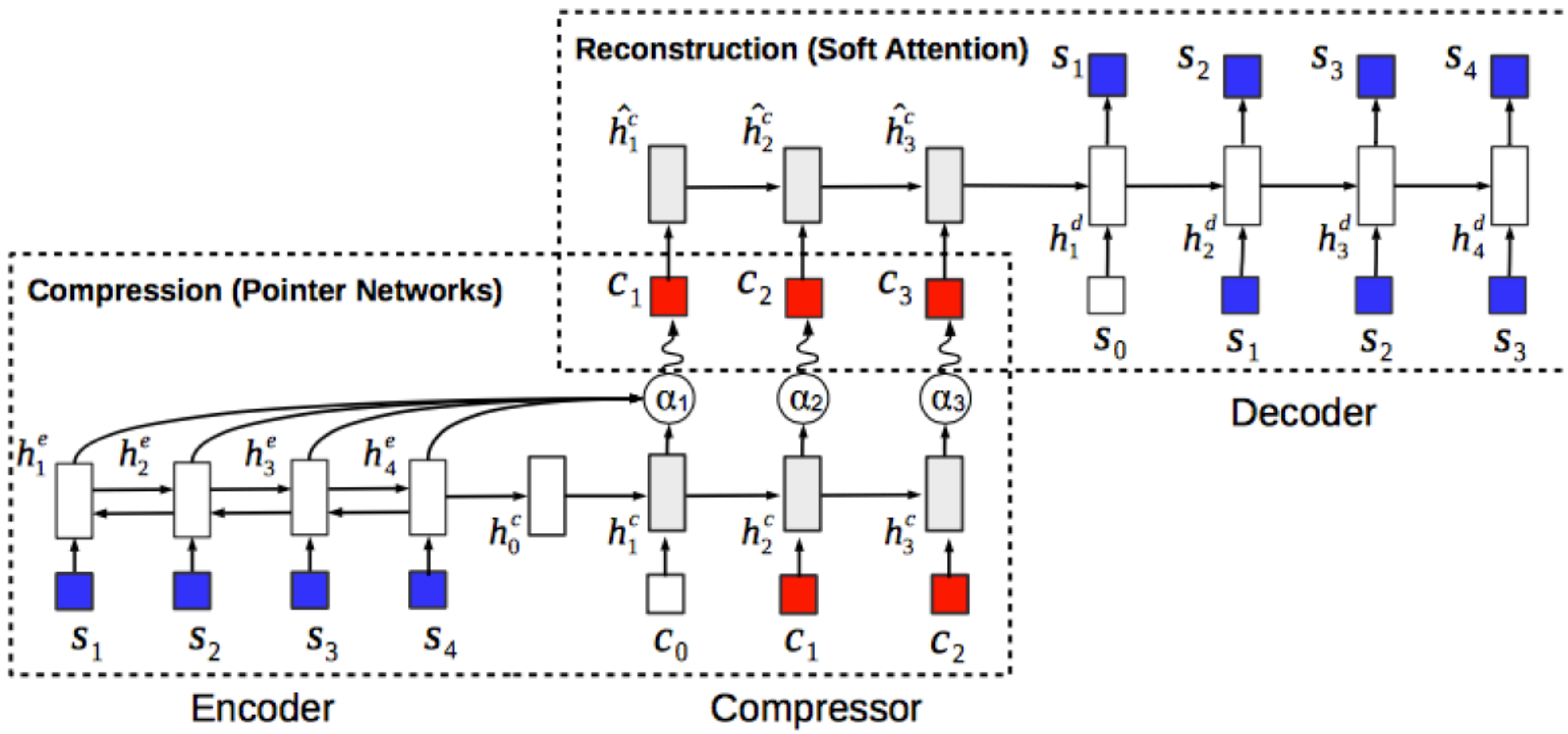
- As τ approaches 0, will approach max



Application Examples in NLP

Symbol Sequence Latent Variables (Miao and Blunsom 2016)

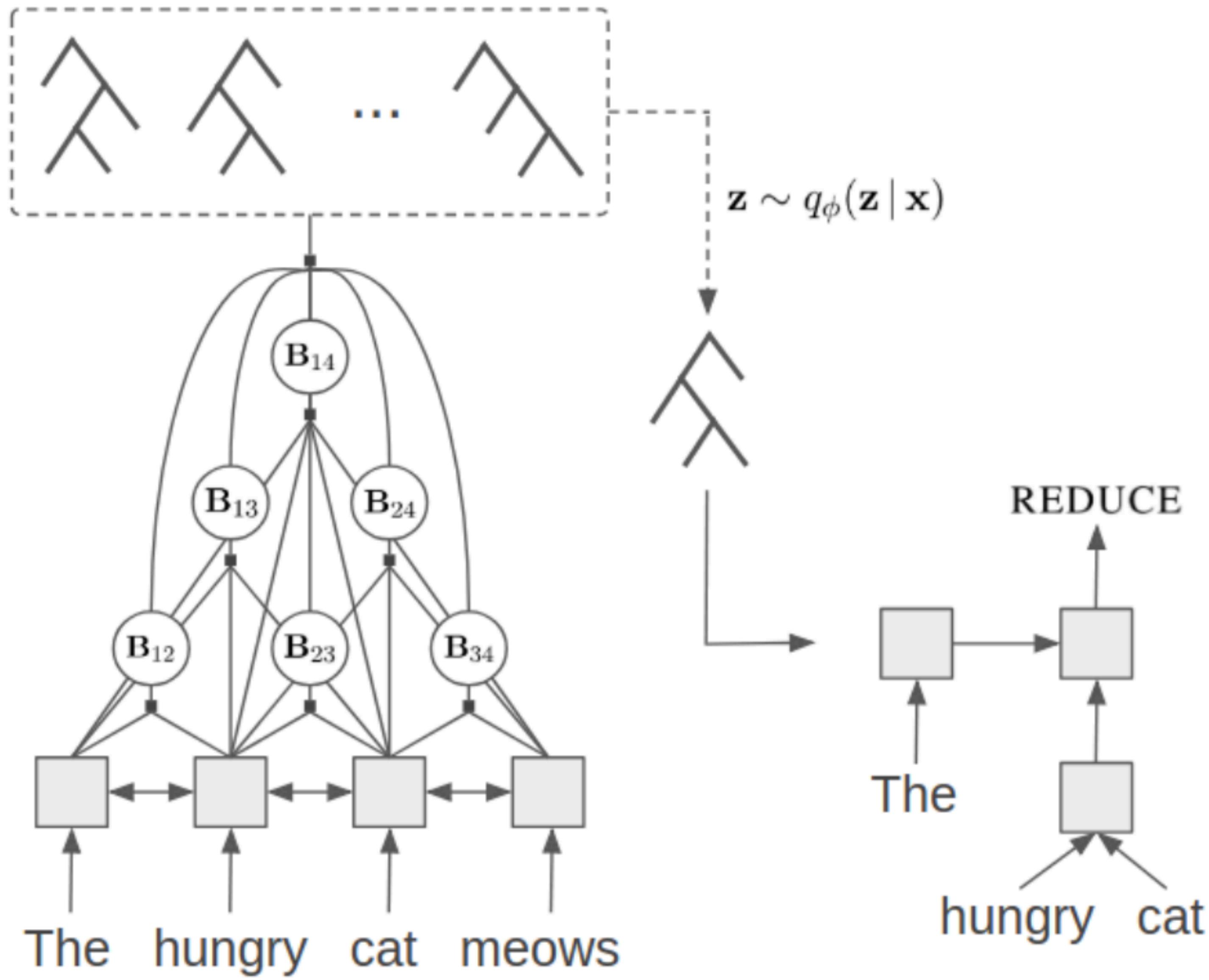
- Encoder-decoder with a sequence of latent symbols



- Summarization in Miao and Blunsom (2016)
- Attempts to "discover" language (e.g. Havrylov and Titov 2017)
    - But things may not be so simple! (Kottur et al. 2017)

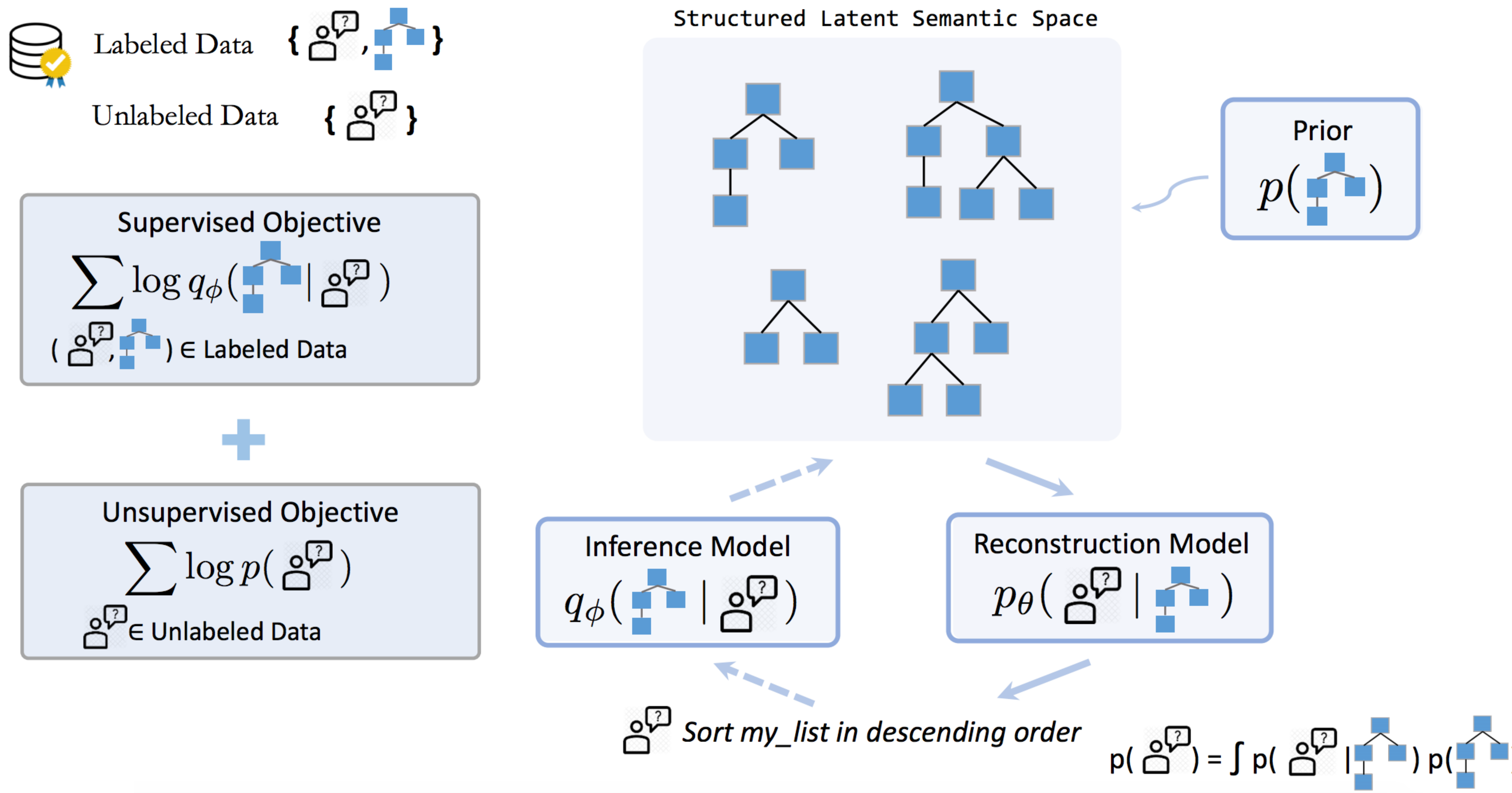
Unsupervised Recurrent Neural Network Grammars

(Kim et al., 2019)



Inference Network $q_\phi(\mathbf{z} \mid \mathbf{x})$ Generative Model $p_\theta(\mathbf{x}, \mathbf{z})$

STRUCTVAE: Tree-structured Latent Variable Models for Semi-supervised Semantic Parsing (Yin et al. 2018)



Questions?