CS11-747 Neural Networks for NLP

Models w/ Latent Random Variables

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Site
https://phontron.com/class/nn4nlp2019/

With Slides from Graham Neubig

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

    - Globally normalized CRF POS tagger

    - Language model

Types of Variables

- Observed vs. Latent:
  - **Observed:** something that we can see from our data, e.g. X or Y
  - **Latent:** a variable that we assume exists, but we aren't given the value
- Deterministic vs. Random:
  - **Deterministic:** variables that are calculated directly according to some deterministic function
  - **Random (stochastic):** variables that obey a probability distribution, and may take any of several (or infinite) values

Quiz: What Types of Variables?

- In the an attentional sequence-to-sequence model using MLE/teacher forcing, are the following variables observed or latent? deterministic or random?
    - The input word ids **f**
    - The encoder hidden states **h**
    - The attention values **a**
    - The output word ids **e**

Latent Variable Models

- A latent variable model (LVM) is a probability distribution over two sets of variables x, z :

$$p(x, z; \theta)$$

where the x variables are observed at learning time in a dataset and z are latent variables.

What is Latent Random Variable Model

- Older latent variable models
  - Topic models (unsupervised)

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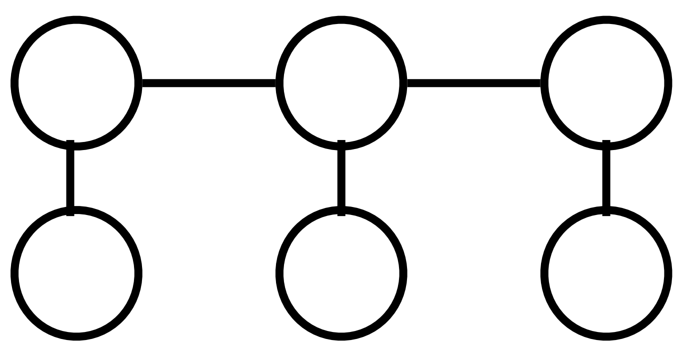
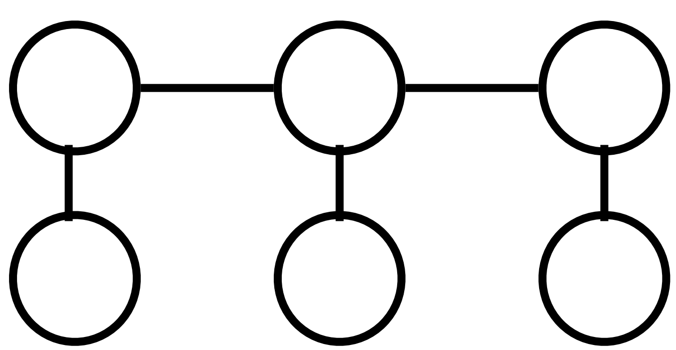
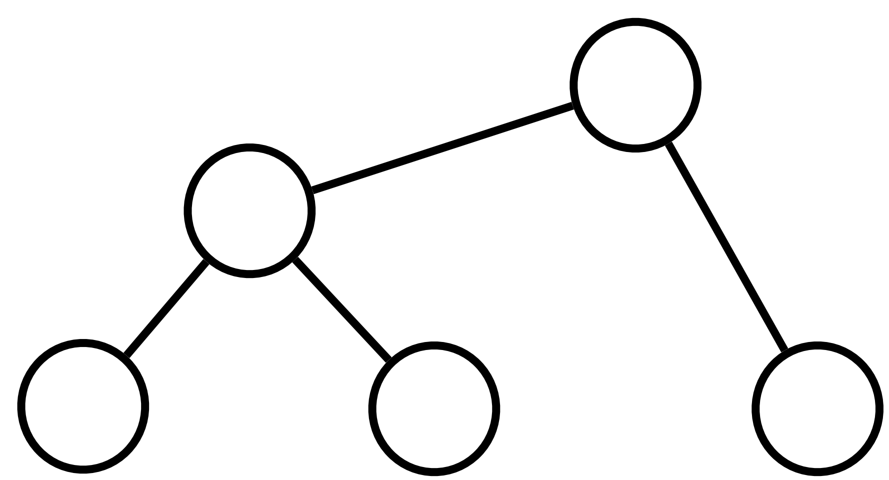
  - Hidden Markov Model (unsupervised tagger)



What is Latent Random Variable Model

- Older latent variable models
  - Topic models (unsupervised)
  - Hidden Markov Model (unsupervised tagger)
  - Some tree-structured Model (unsupervised parsing)





Why Latent Variable Models?

- Some variables are not observed naturally and we want to model / infer these hidden variables: e.g. topics of an article

- Specify structural relationships in the context of unknown variables, to learn interpretable structure:
  - Inject inductive bias / prior knowledge

Deep Structured Latent Variable Models

- Specify structure, but interpretable structure is often discrete: e.g. POS tags, dependency parse trees

- There is always a tradeoff between interpretability and flexibility: model constraints v.s. model capacity

Examples of Deep Latent Variable Models

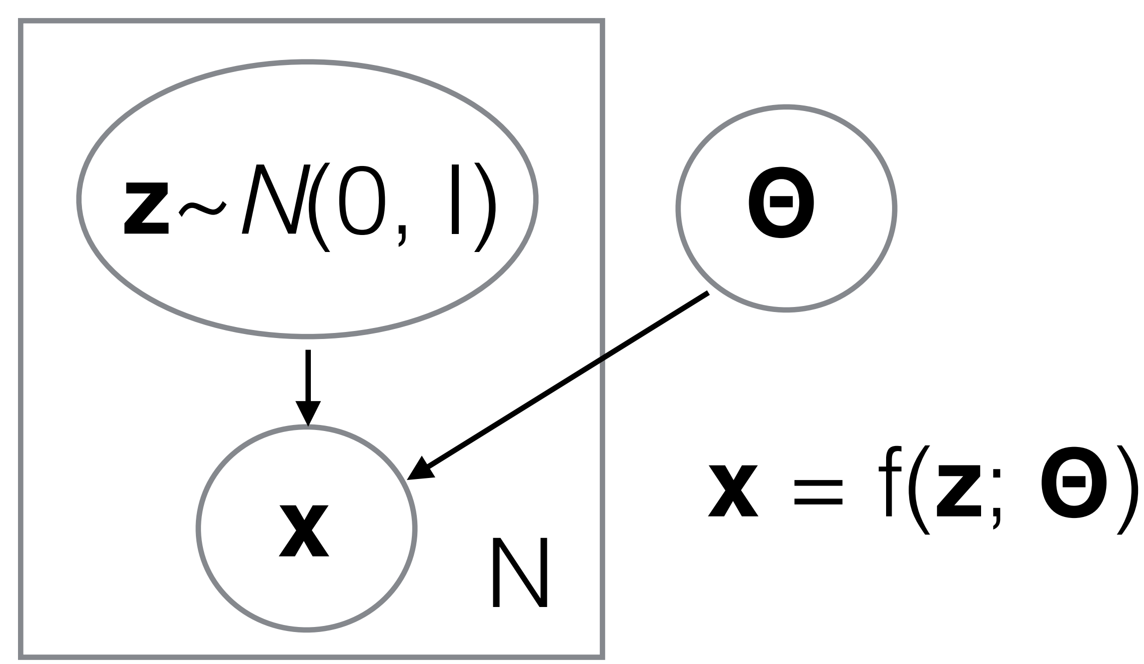
- Deep latent variable models
  - Variational Autoencoders (VAEs)
  - Generative Adversarial Network (GANs)
  - Flow-based generative models

Variational Auto-encoders

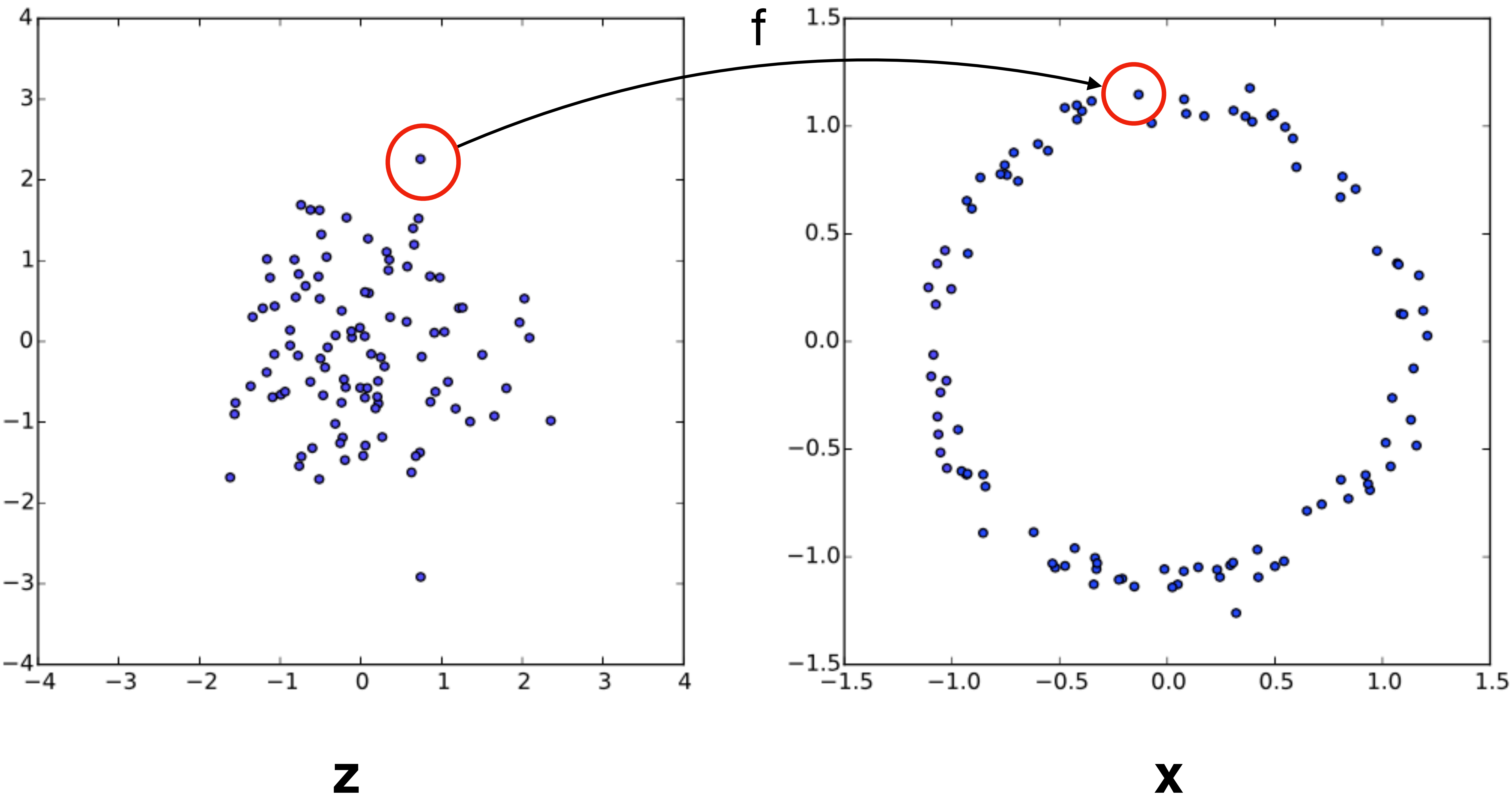
(Kingma and Welling 2014)

A Latent Variable Model

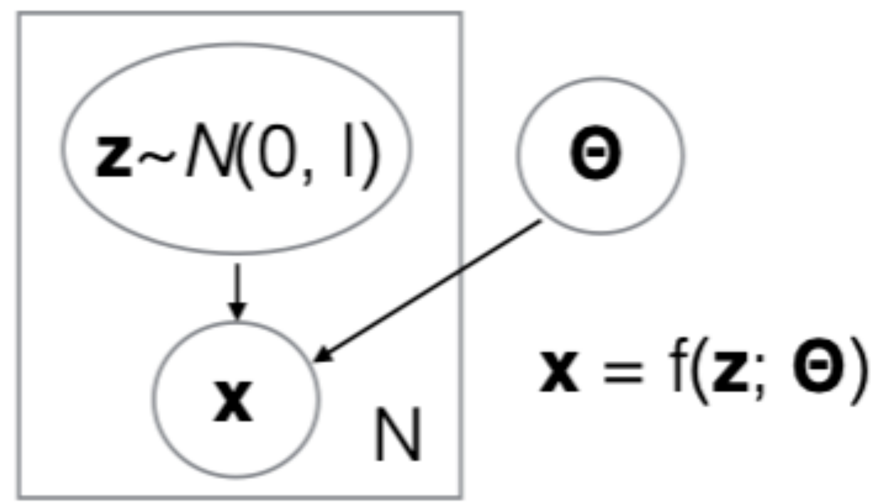
- We observed output **x** (assume a continuous vector for now)
- We have a latent variable **z** generated from a Gaussian
- We have a function f, parameterized by **Θ** that maps from **z** to **x**, where this function is usually a neural net



An Example (Goersch 2016)



A probabilistic perspective on Variational Auto-Encoder



- 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:

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

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

- Variational inference approximates the posterior 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 $q_\phi(z|x)$

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

- Variational Lower Bound (ELBO)

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

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

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

Variational Inference

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

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

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 (z|x), but the lower bound is tight only if q(z|x) = p(z|x)

p(z|x) is intractable

Practice

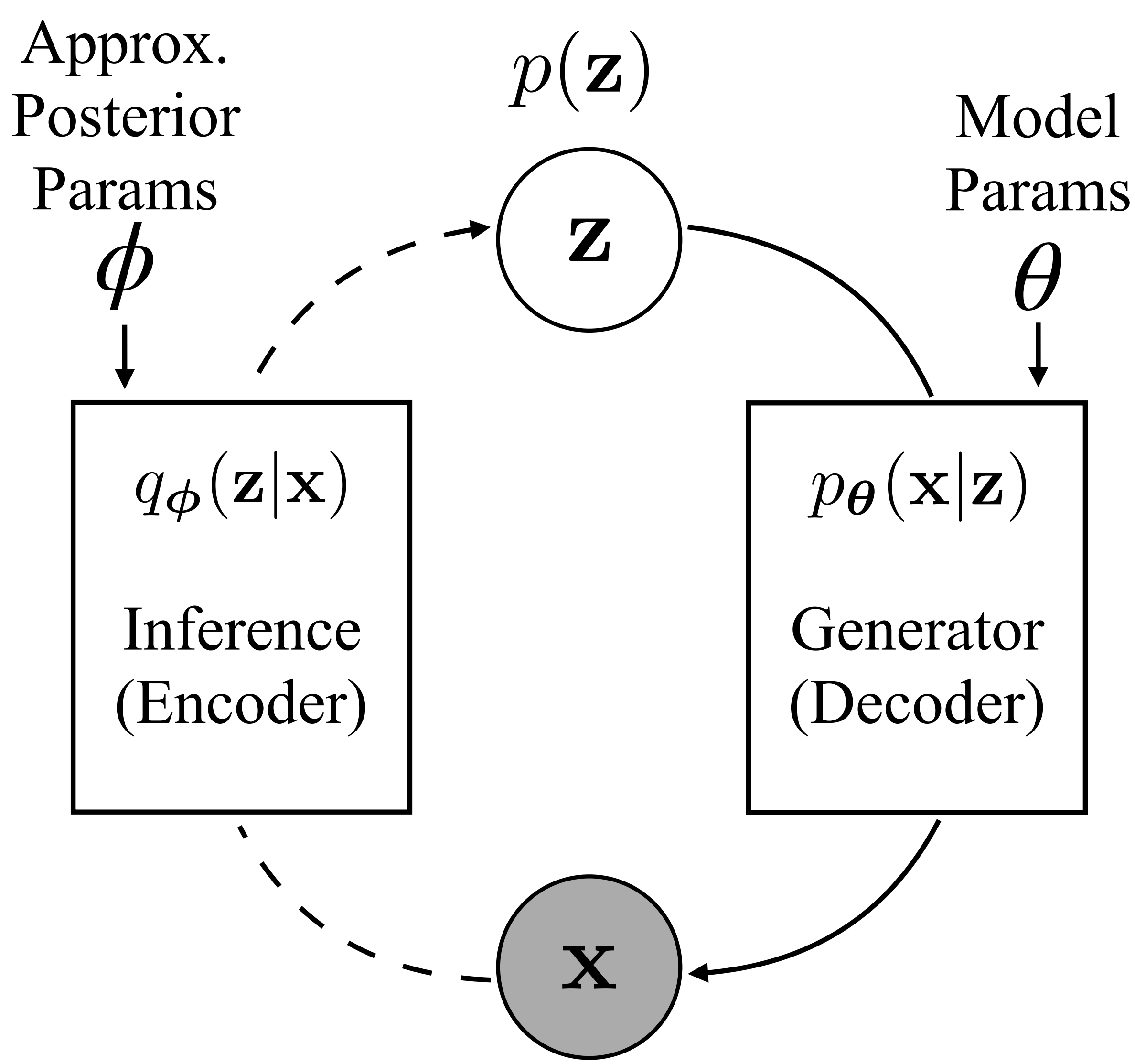
Prove

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

Hint: use Jensen's inequality

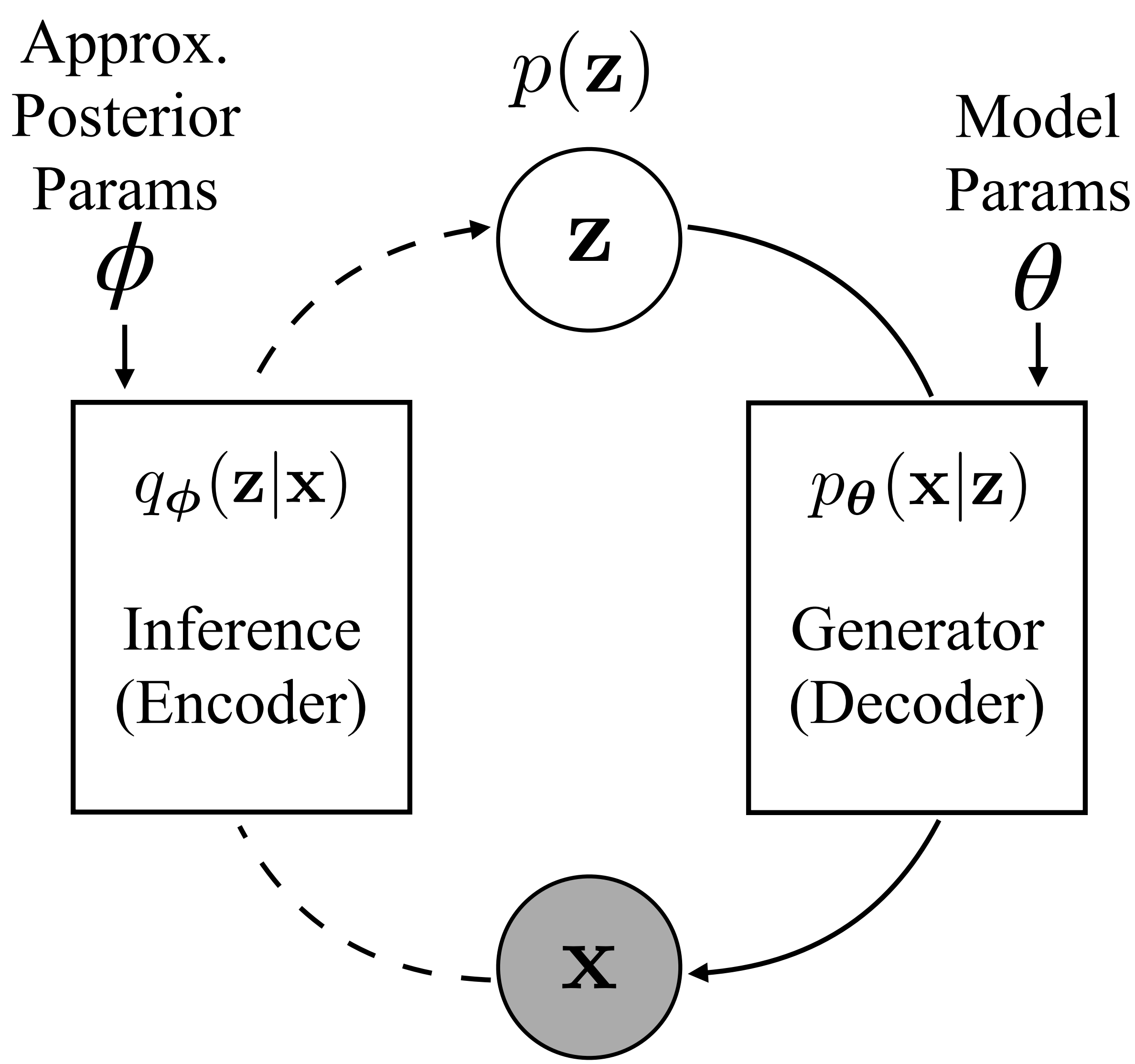
Variational Autoencoders

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



Variational Autoencoders

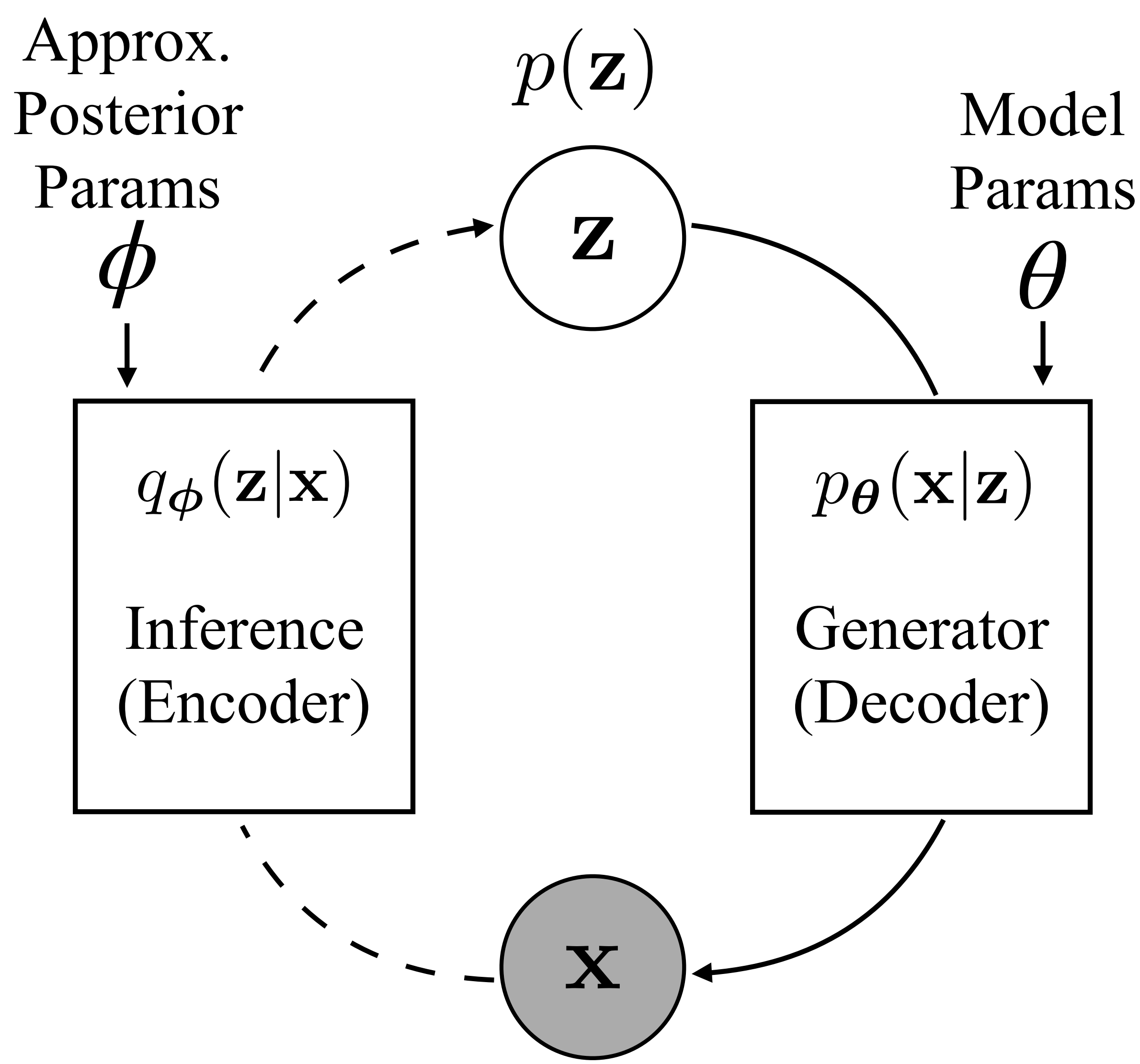
$$\log p_{\boldsymbol{\theta}}(\mathbf{x}) >= \underbrace{\mathbb{E}_{\mathbf{z}\sim q_{\phi}(\mathbf{z}|\mathbf{x})}[\log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})]}_{\text{Reconstruction Loss}} - \underbrace{D_{\mathrm{KL}}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})\|p(\mathbf{z}))}_{\text{KL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



Regularized Autoencoder

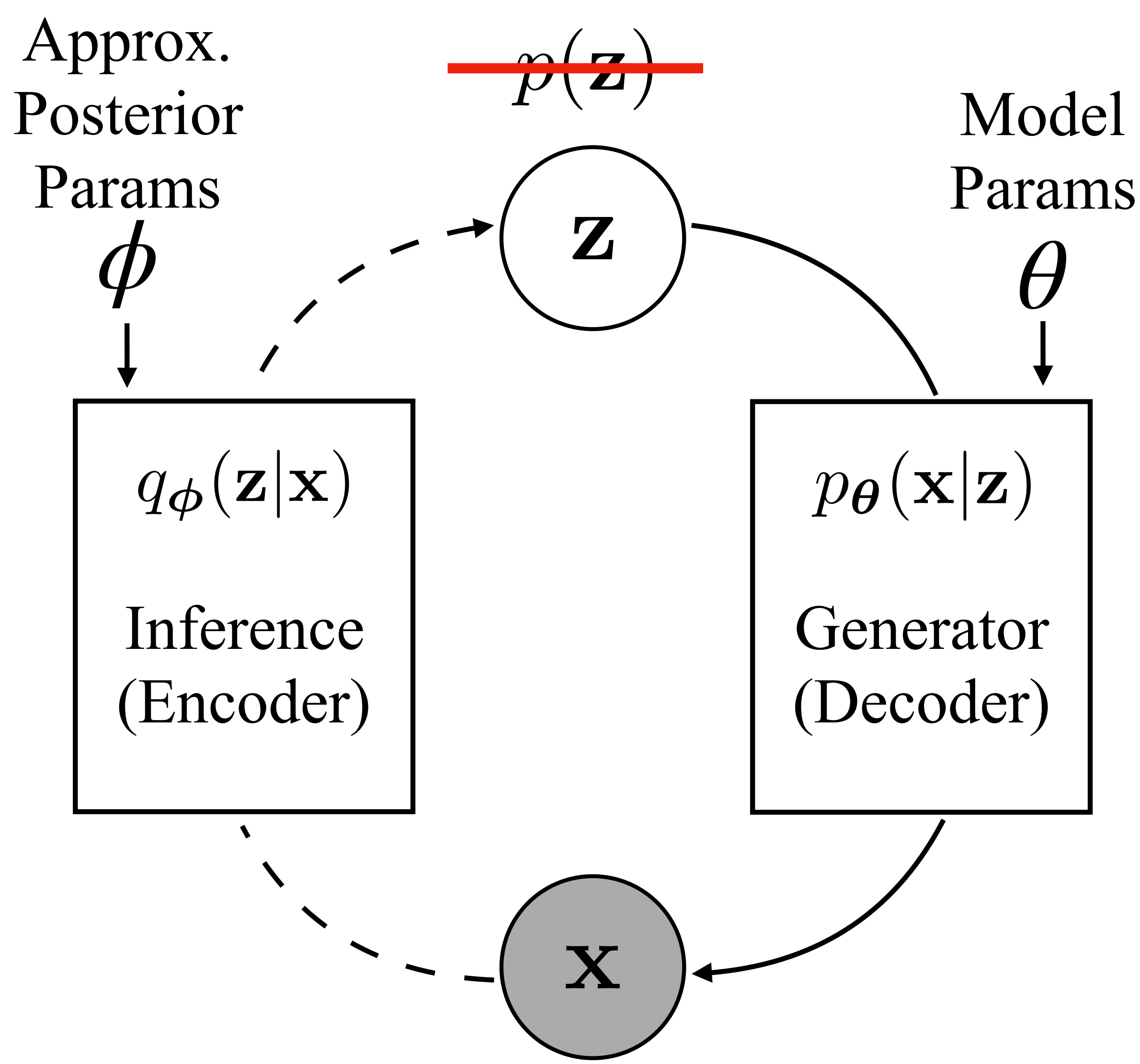
Why prior ?

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



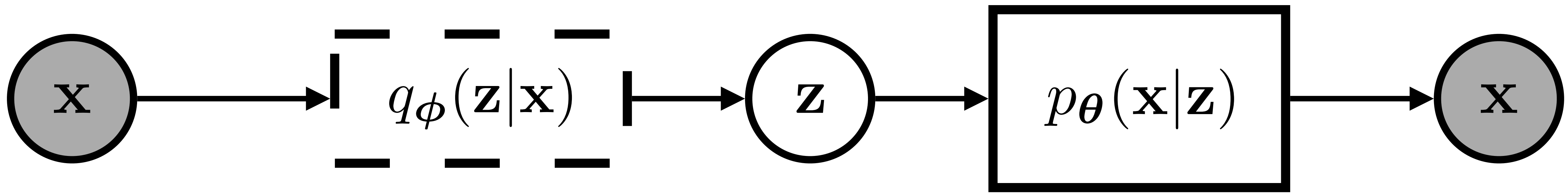
Why prior ?

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



VAE vs. AE

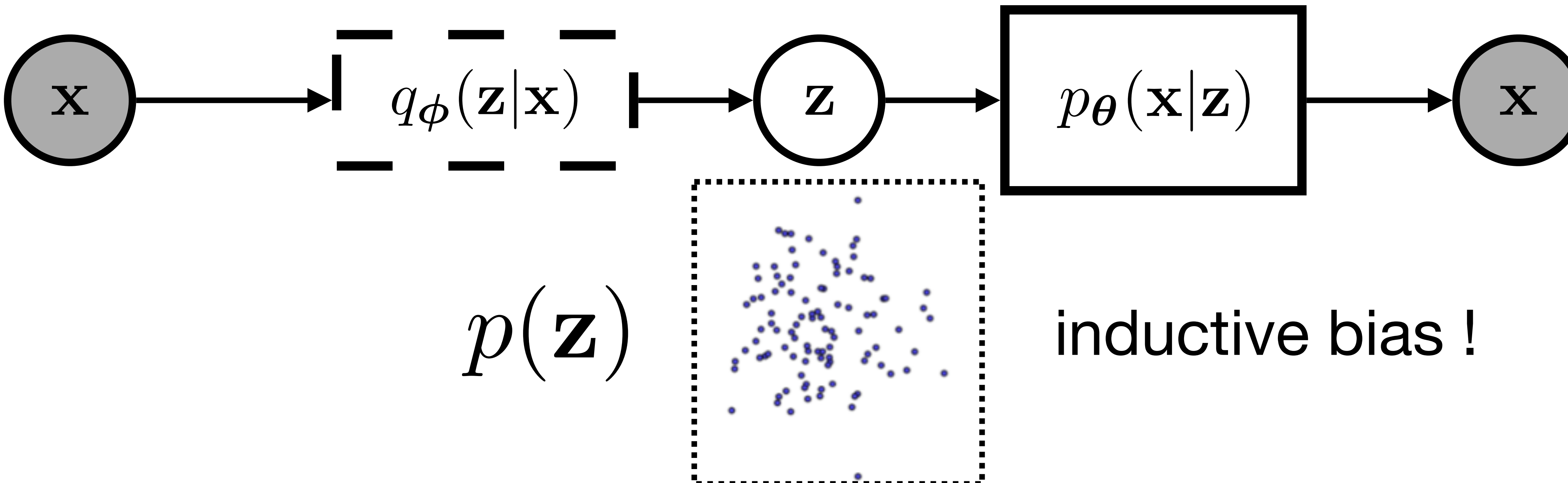
VAE



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

VAE vs. AE

VAE



inductive bias !

VAE vs. AE

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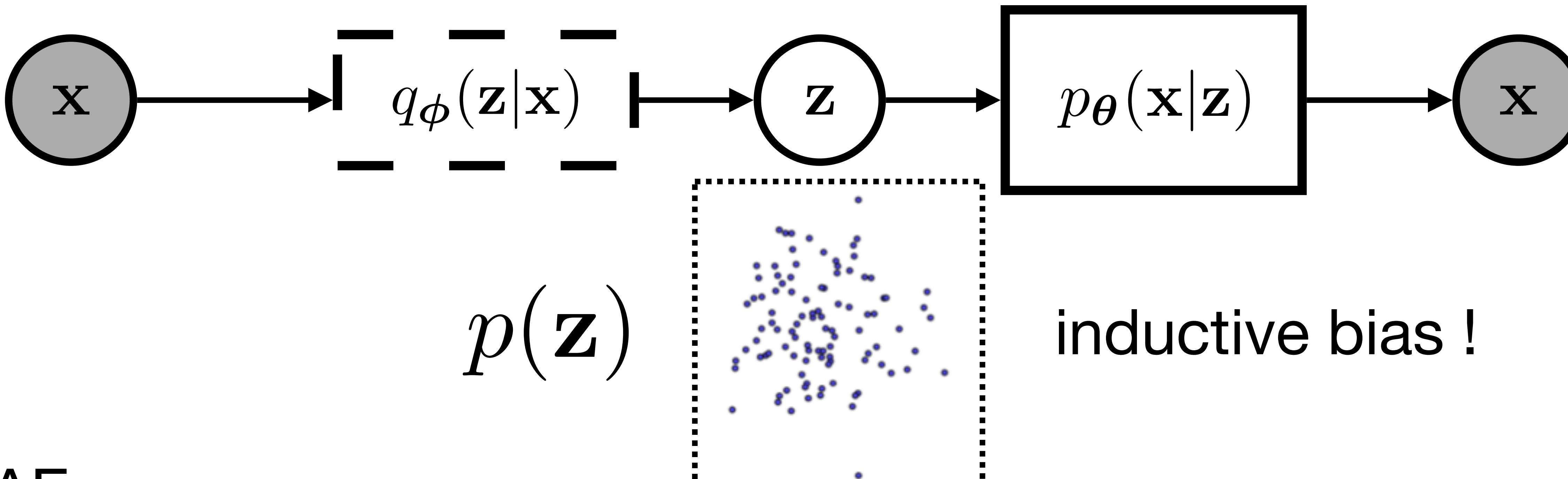

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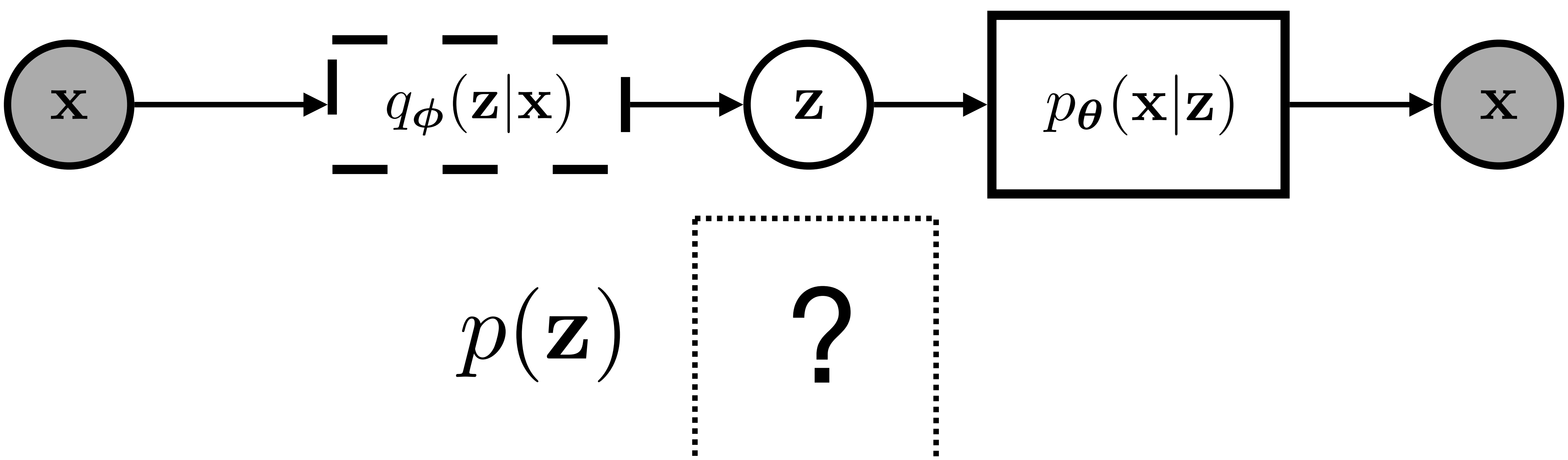

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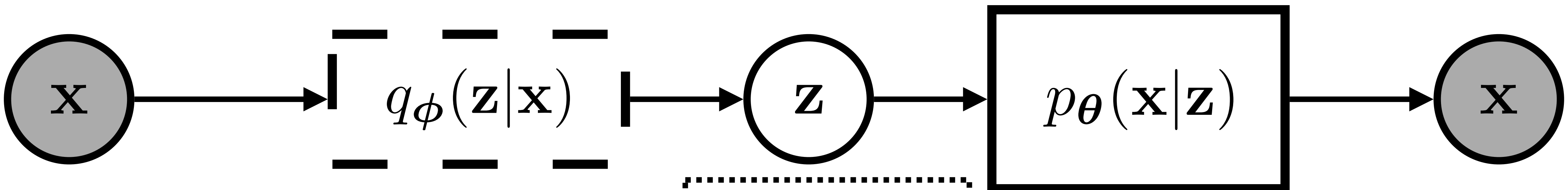
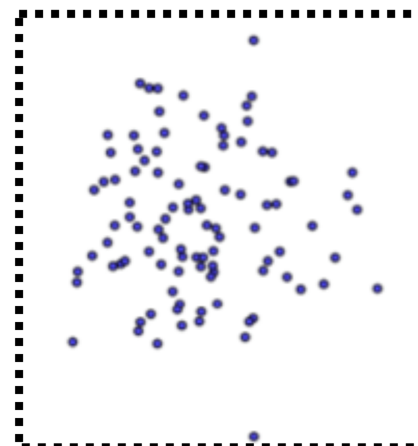


$p(\mathbf{z})$



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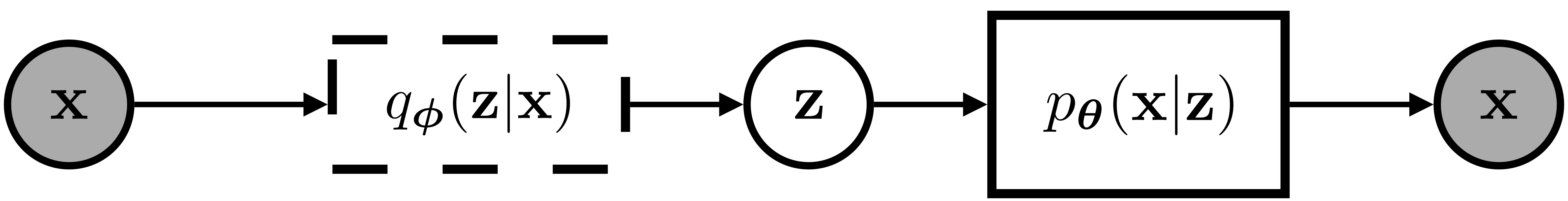
AE



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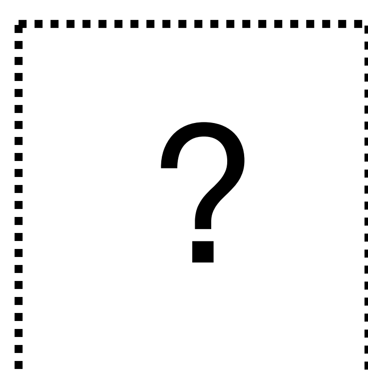

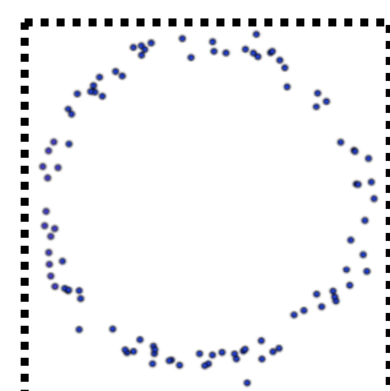

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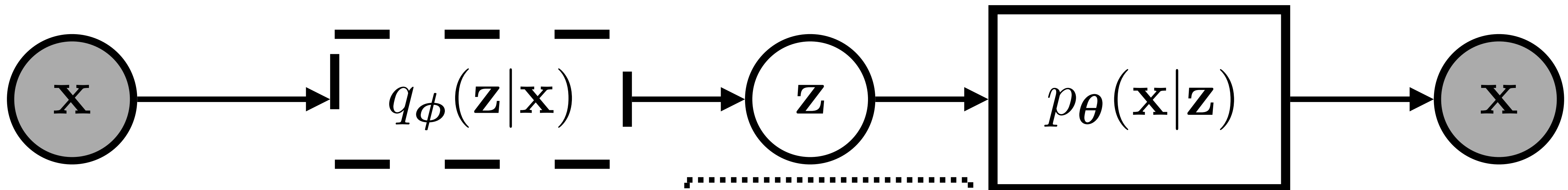

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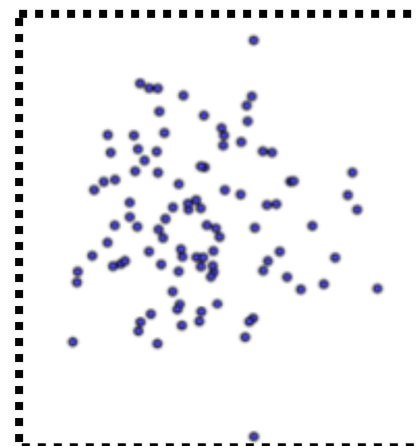

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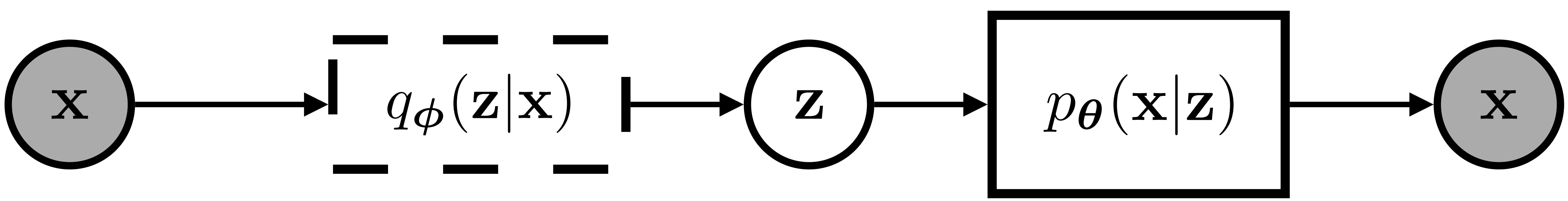
AE



AE is not generative model:

1. Can't sample new data from AE
2. Can't compute the log likelihood of data x

Why VAE

- Generative modeling
- Representation learning
  - Representation space can be regularized by prior
- Unsupervised learning

Why VAE

	VAE	AE		
Generative modeling	Yes	No		
Representation Learning	Yes	Yes		
Unsupervised Learning	Yes	Yes		
Controlled representation space	Yes	No		

Why VAE

	VAE	AE	LSTM LM	
Generative modeling	Yes	No		
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Representation Learning	Yes	Yes	Yes	
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Why VAE

	VAE	AE	LSTM LM	CNN Classifier
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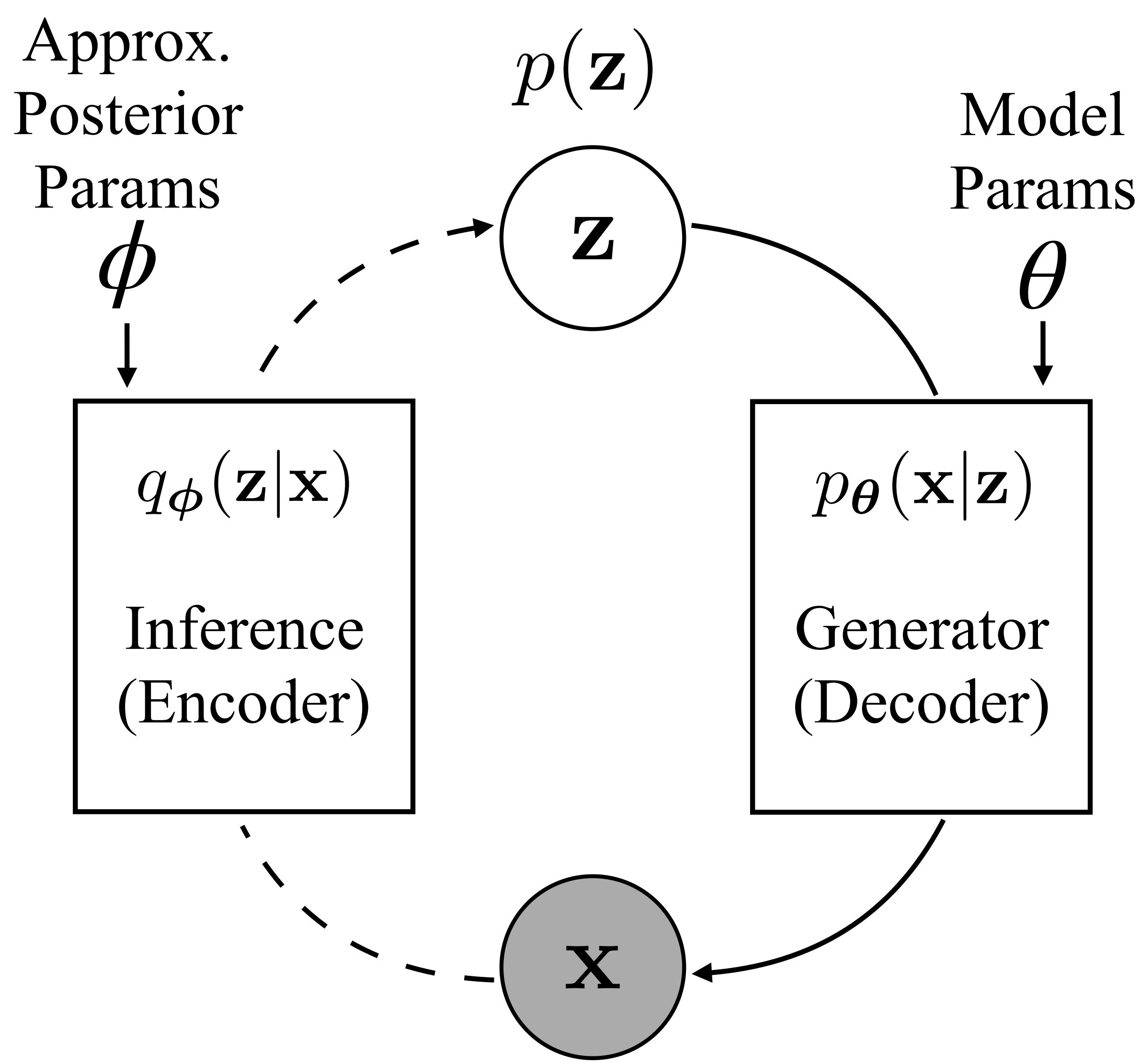
Representation Learning	Yes	Yes	Yes	
Unsupervised Learning	Yes	Yes	Yes	
Controlled representation space	Yes	No	No	

Why VAE

	VAE	AE	LSTM LM	CNN Classifier
Generative modeling	Yes	No	Yes	No
Representation Learning	Yes	Yes	Yes	Yes
Unsupervised Learning	Yes	Yes	Yes	No
Controlled representation space	Yes	No	No	No

Learning 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

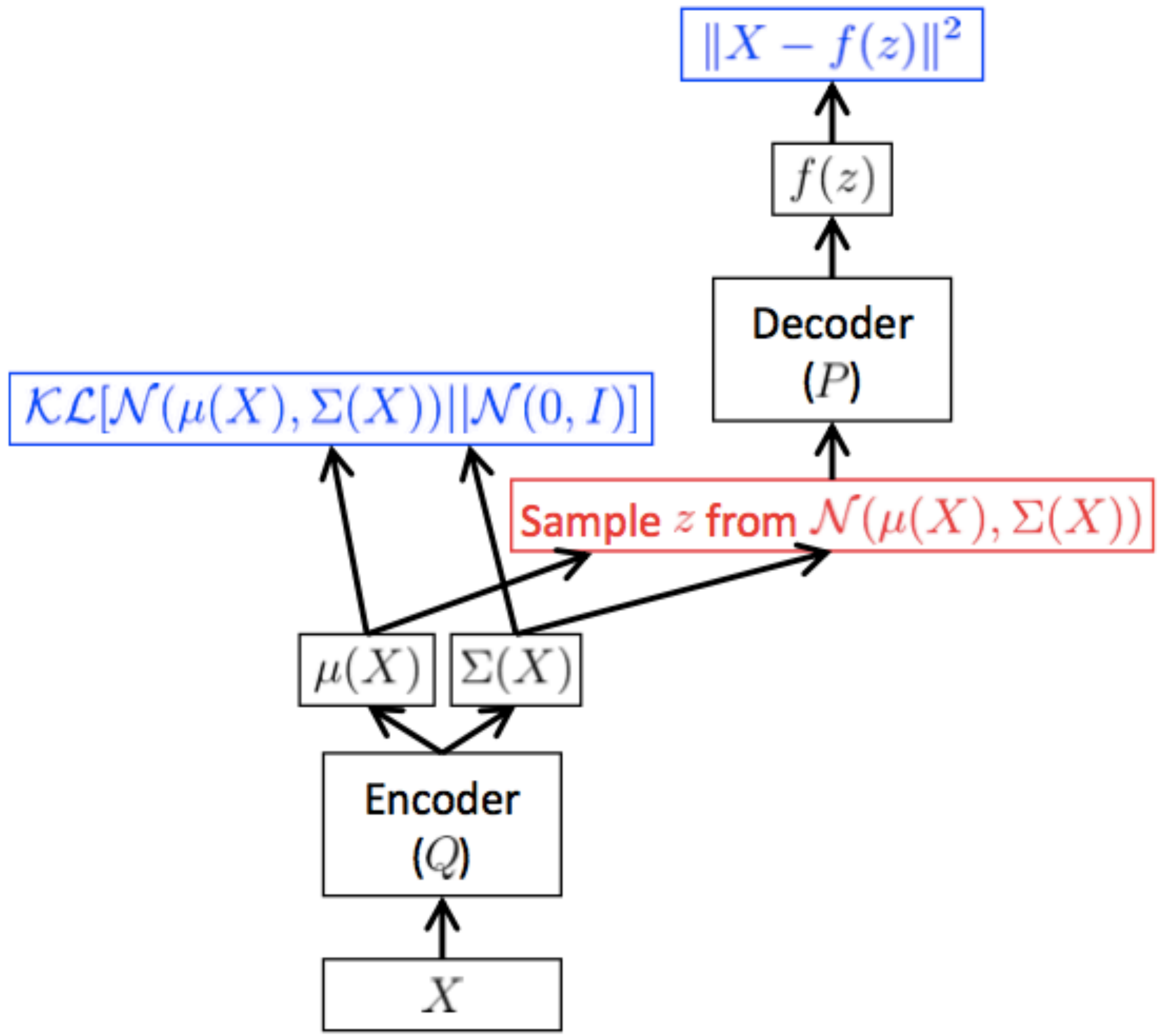


Figure Credit: Doersch (2016)

Solution: Re-parameterization Trick

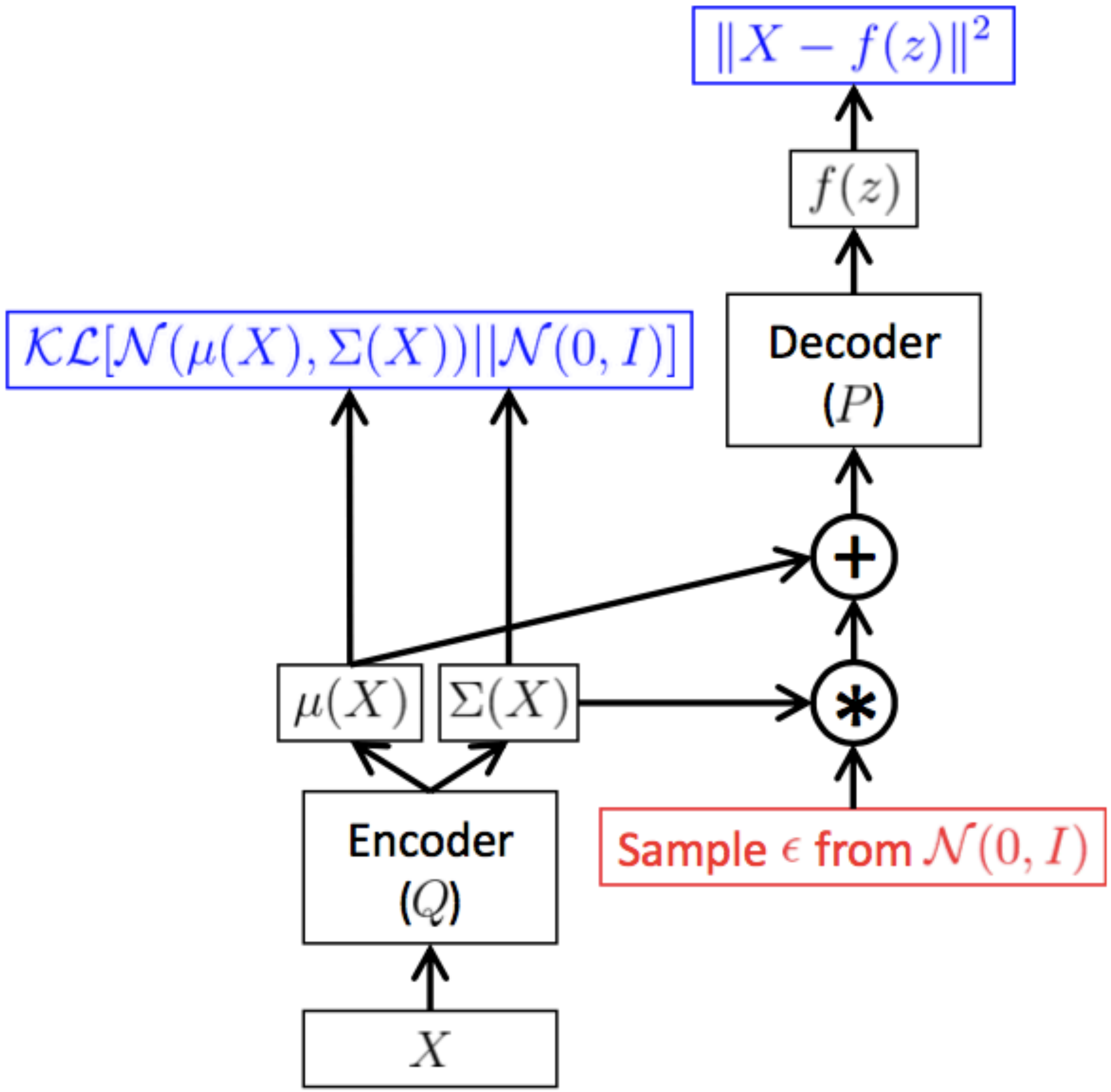


Figure Credit: Doersch (2016)

An Example: Generating Sentences w/ Variational Autoencoders

Generating from Language Models

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

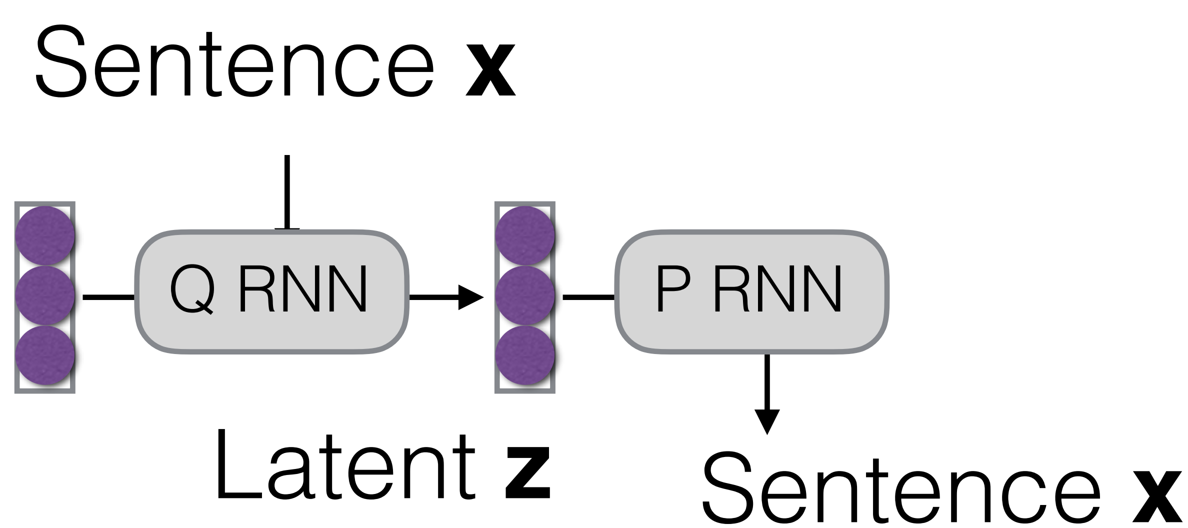
```
while x_{j-1} != "</s>":
  x_j ~ P(x_j | x_1, …, x_{j-1})
```

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

```
while y_{j-1} != "</s>":
  y_j ~ P(y_j | X, y_1, …, 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

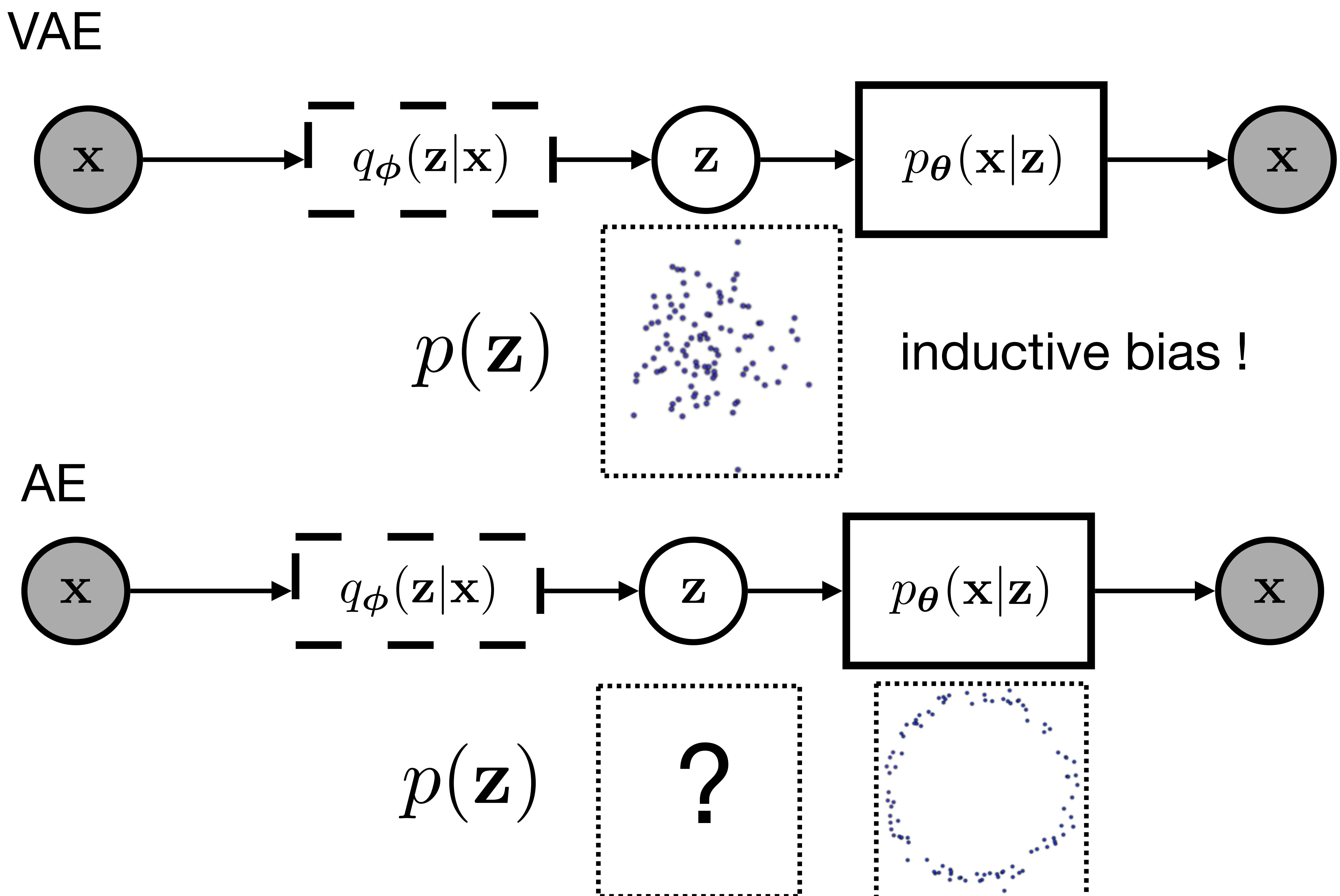
i went to the store to buy some groceries .
i store to buy some groceries .
i were to buy any groceries .
horses are to buy any groceries .
horses are to buy any animal .
horses the favorite any animal .
horses the favorite favorite animal .
horses are my favorite animal .

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.

VAE vs. AE


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

Let’s Try it Out!

`vae-lm.py`

Difficulties in Training

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

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

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

- 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

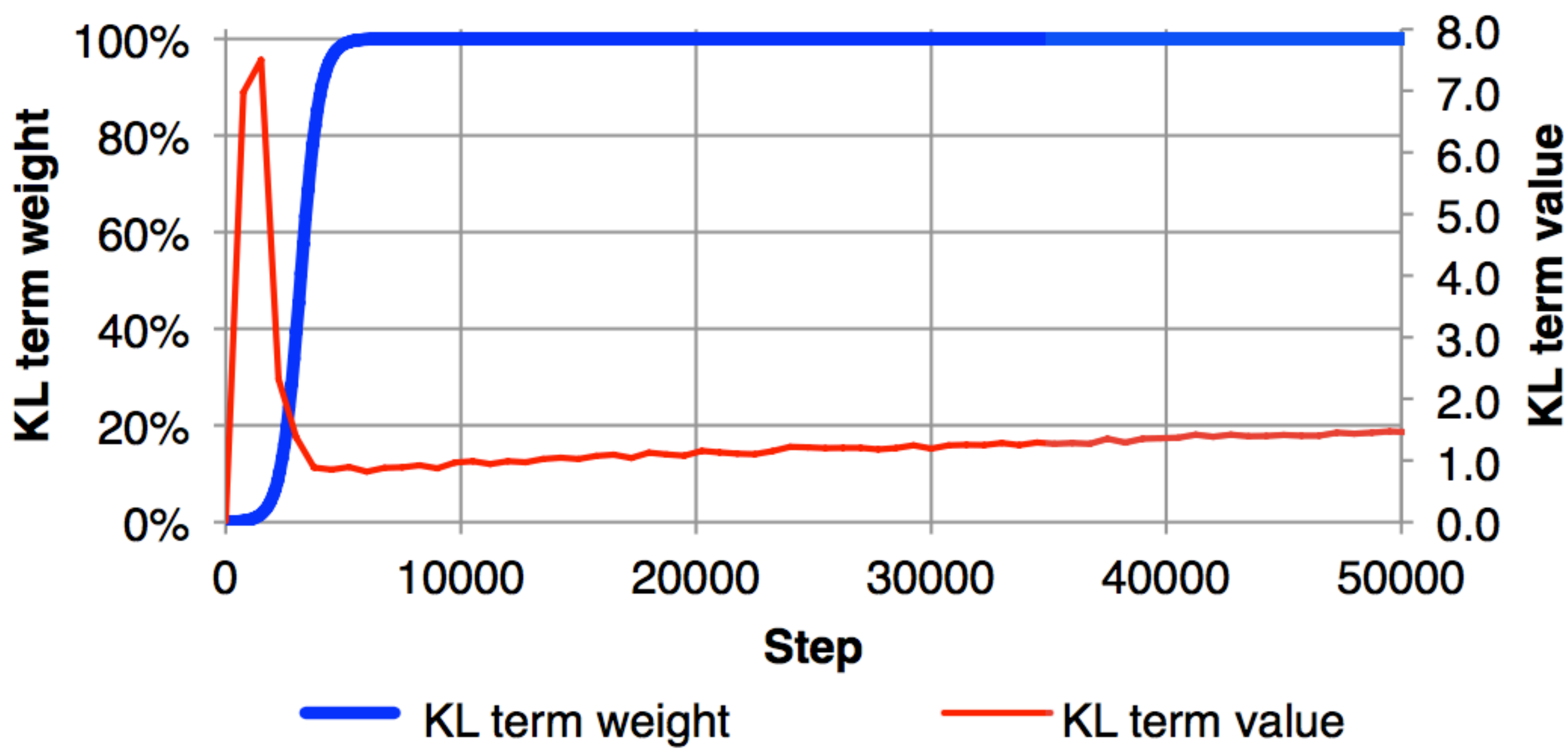


Figure Credit: Bowman et al. (2017)

Solution 2: Free bits / KL thresholding

- Free bits replaces the KL term in ELBO with a hinge loss that maxes 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

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

$$\downarrow$$

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

(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!

<u>Original Categorical Sampling Method:</u>

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

<u>Reparameterized Method</u>

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

where the Gumbel distribution is

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

- Backprop is still not possible, due to argmax

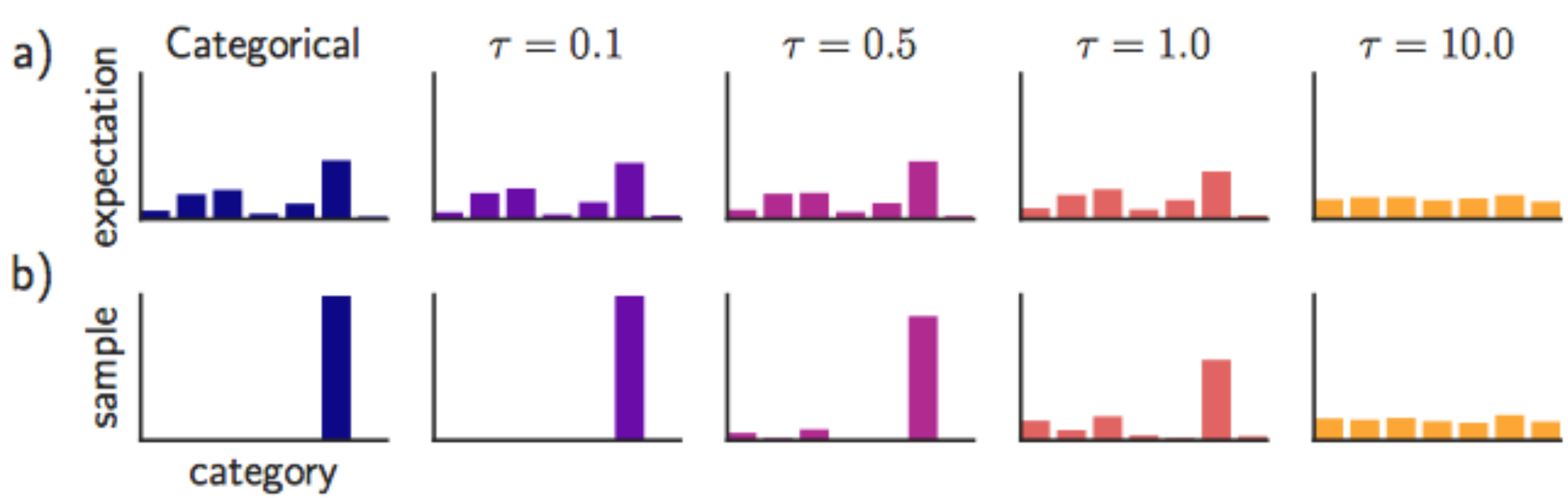
Gumbel-Softmax

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

- Instead of argmax, take softmax with temperature τ

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

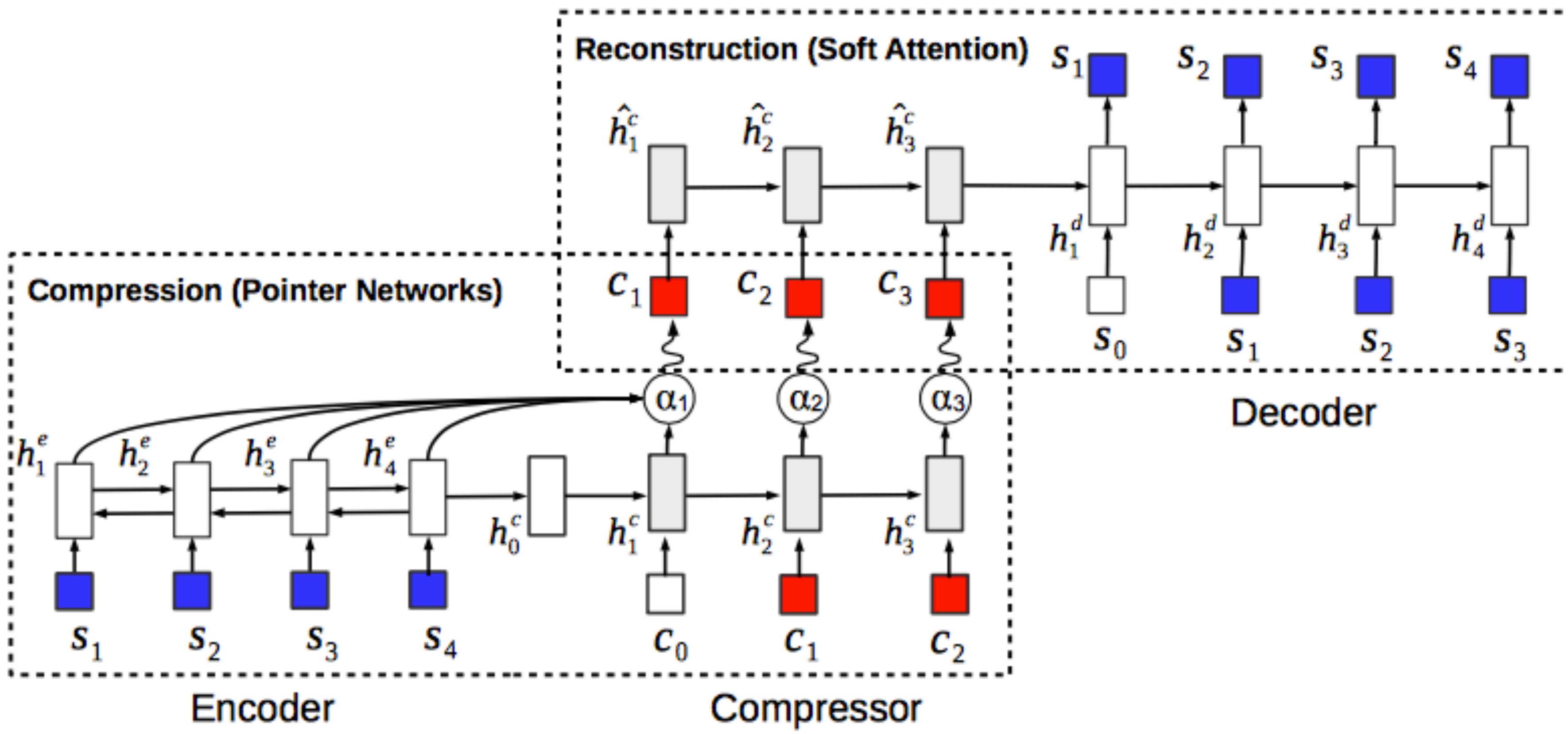
- As τ approaches 0, will approach max



Application Examples in NLP

Symbol Sequence Latent Variables (Miao and Blunsom 2016)

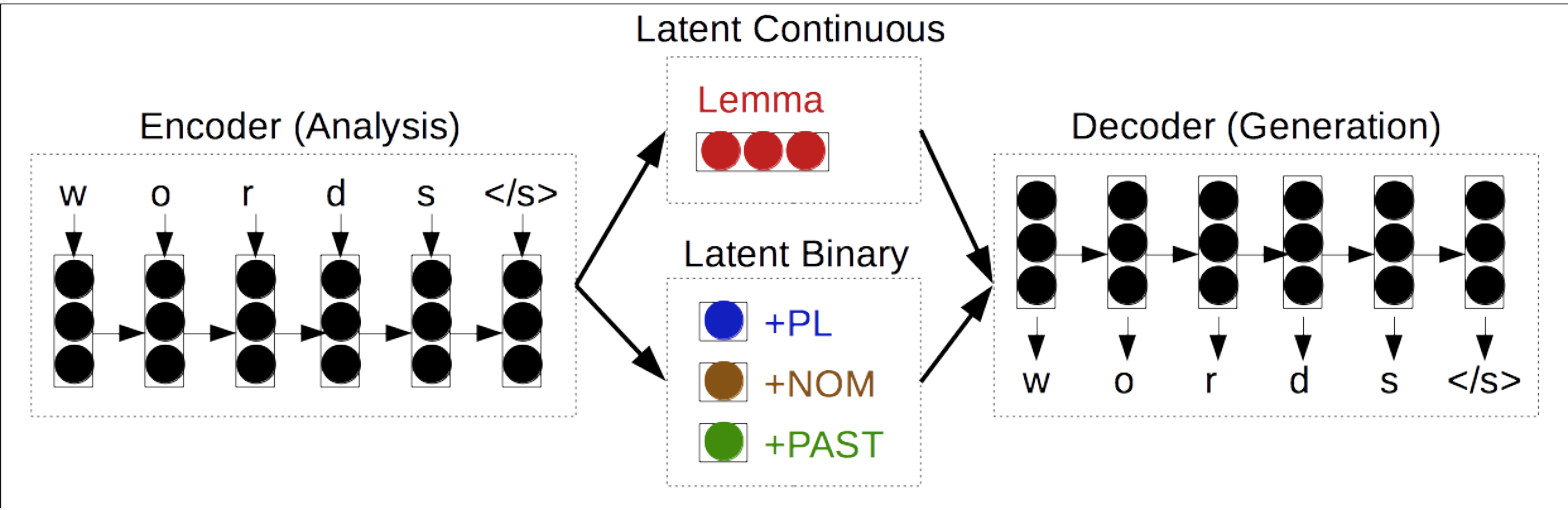
- Encoder-decoder with a sequence of latent symbols



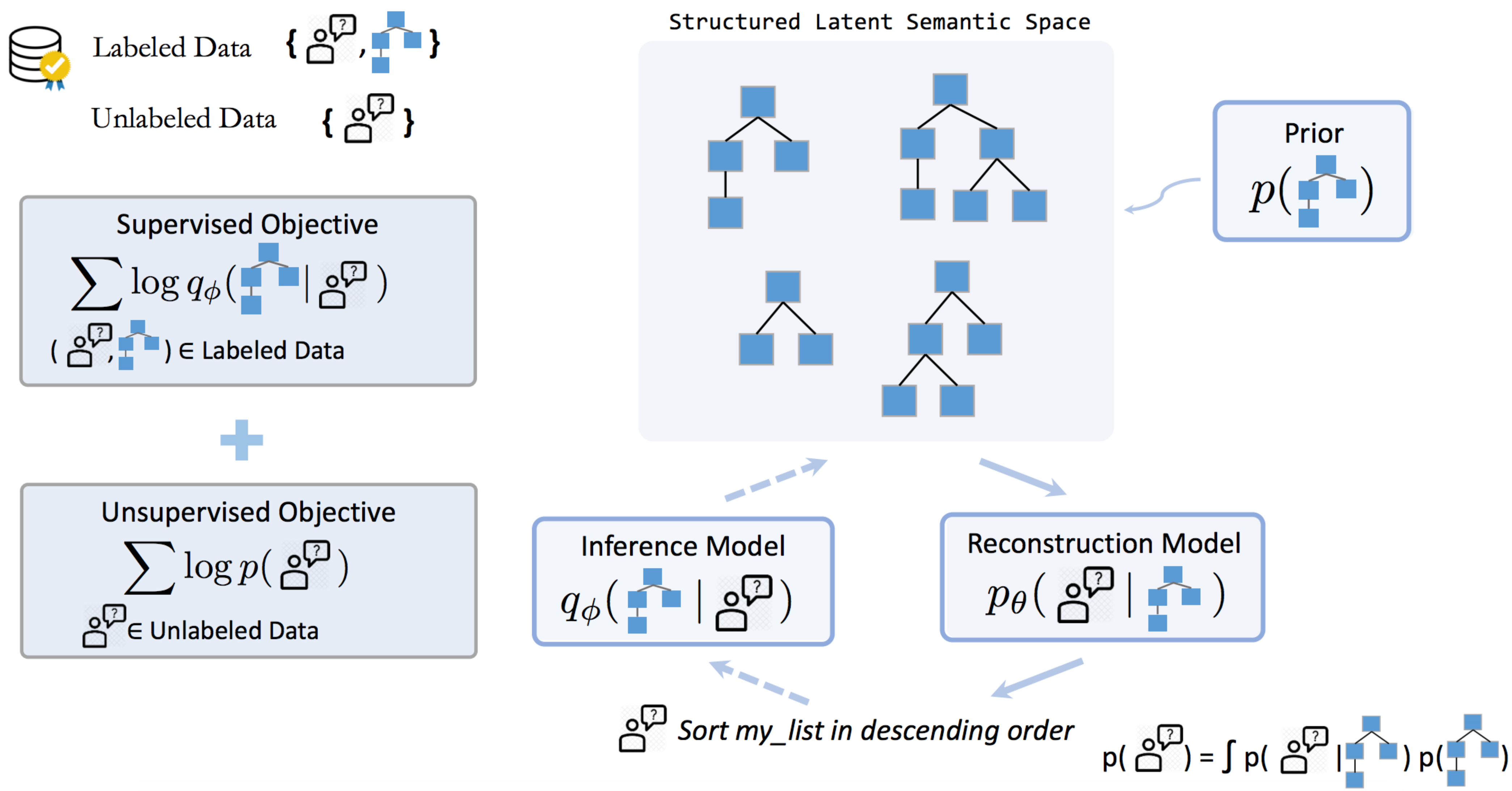
- Summarization in Miao and Blunsom (2016)
- Attempts to “discover” language (e.g. Havrylov and Titov 2017)
  - But things may not be so simple! (Kottur et al. 2017)

Controllable Sequence-to-sequence
(Zhou and Neubig 2017)

- Latent continuous and discrete variables can be trained using auto-encoding or encoder-decoder objective

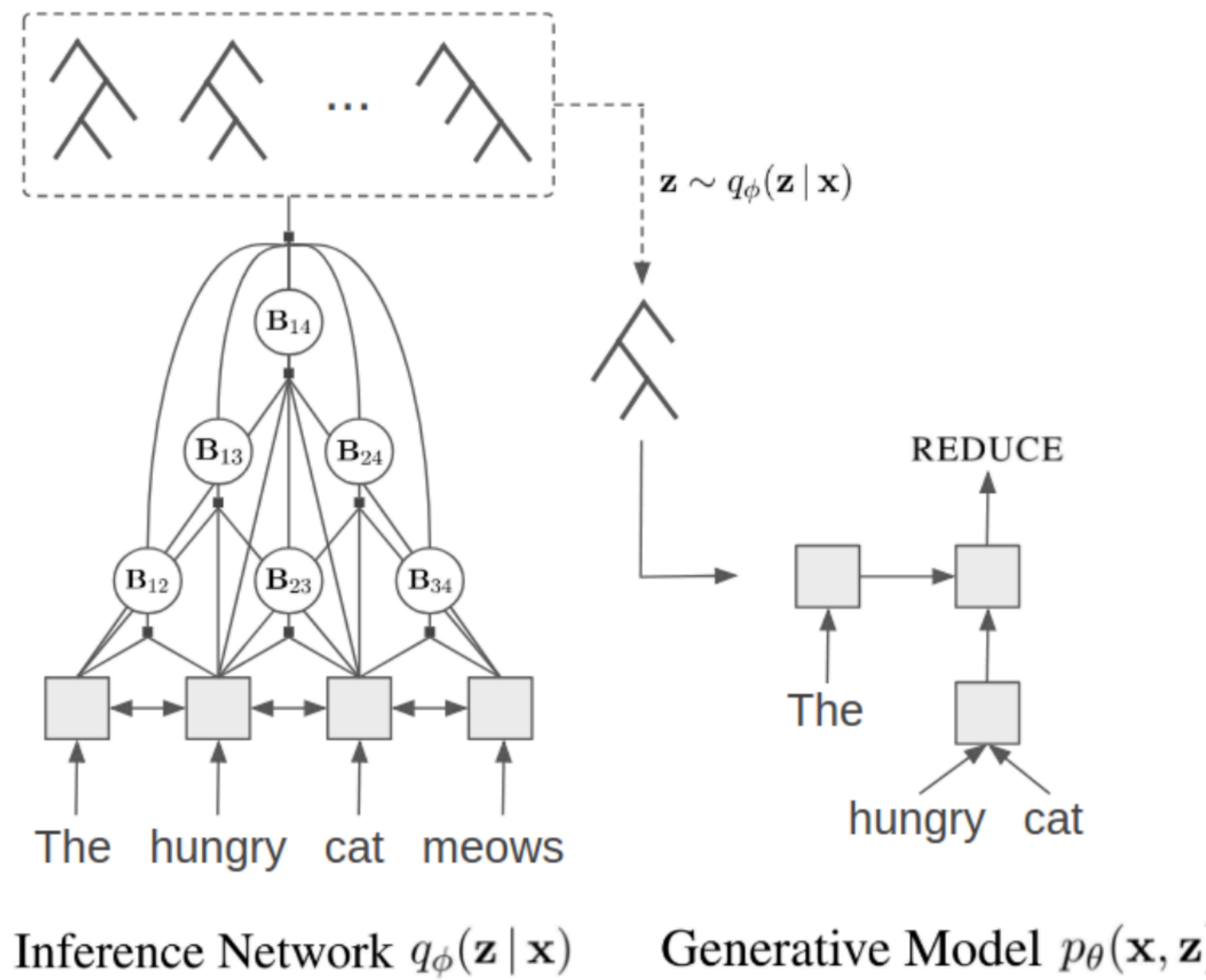


STRUCTVAE: Tree-structured Latent Variable Models for Semi-supervised Semantic Parsing (Yin et al. 2018)



Unsupervised Recurrent Neural Network Grammars

(Kim et al., 2019)



Questions?