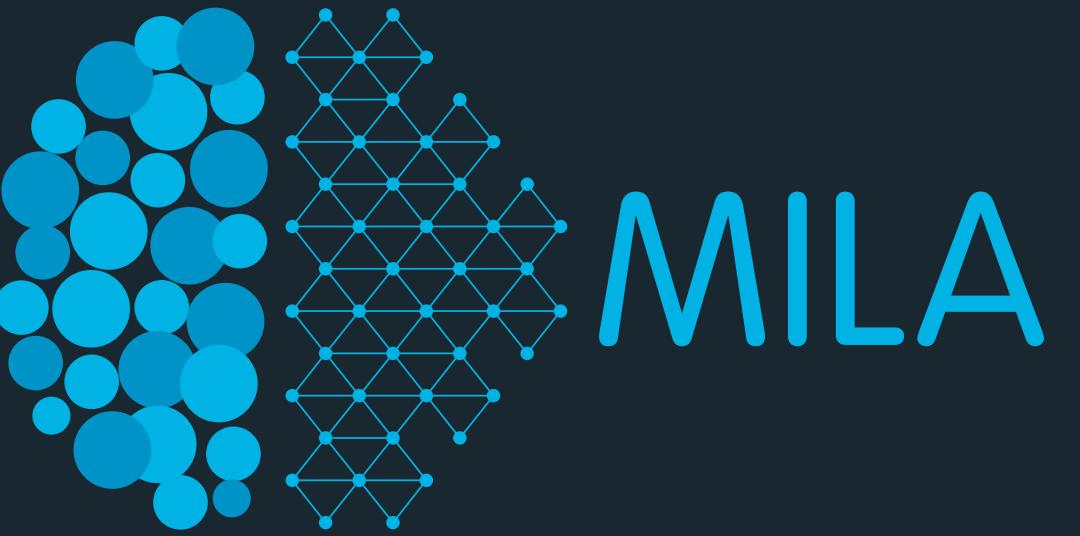


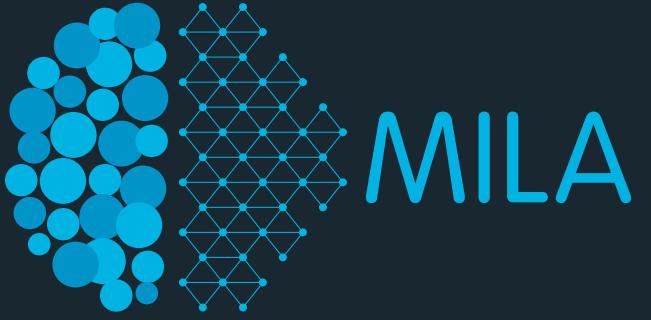
Institut  
des algorithmes  
d'apprentissage  
de Montréal



# Variational Autoencoders

Chin-Wei Huang

# Autoencoders as Generative Models



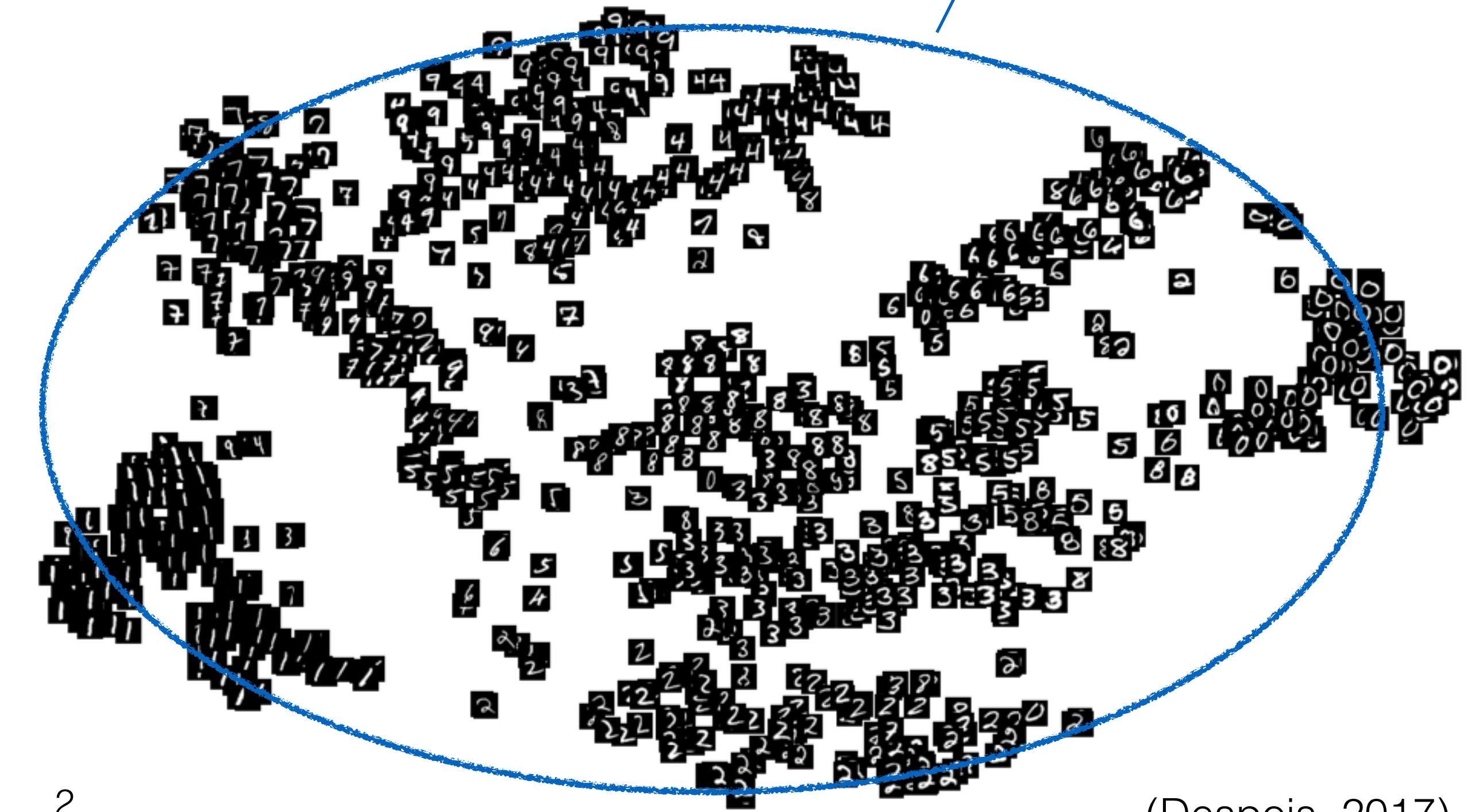
- Regularized autoencoder's objective:

$$\sum_{i=1}^N \underbrace{l(h_\theta(g_\phi(x_i)), x_i)}_{\text{reconstruction term}} + \lambda \overbrace{\Omega(\phi, \theta, g(x_i))}^{\text{regularization term}}$$

parameters →

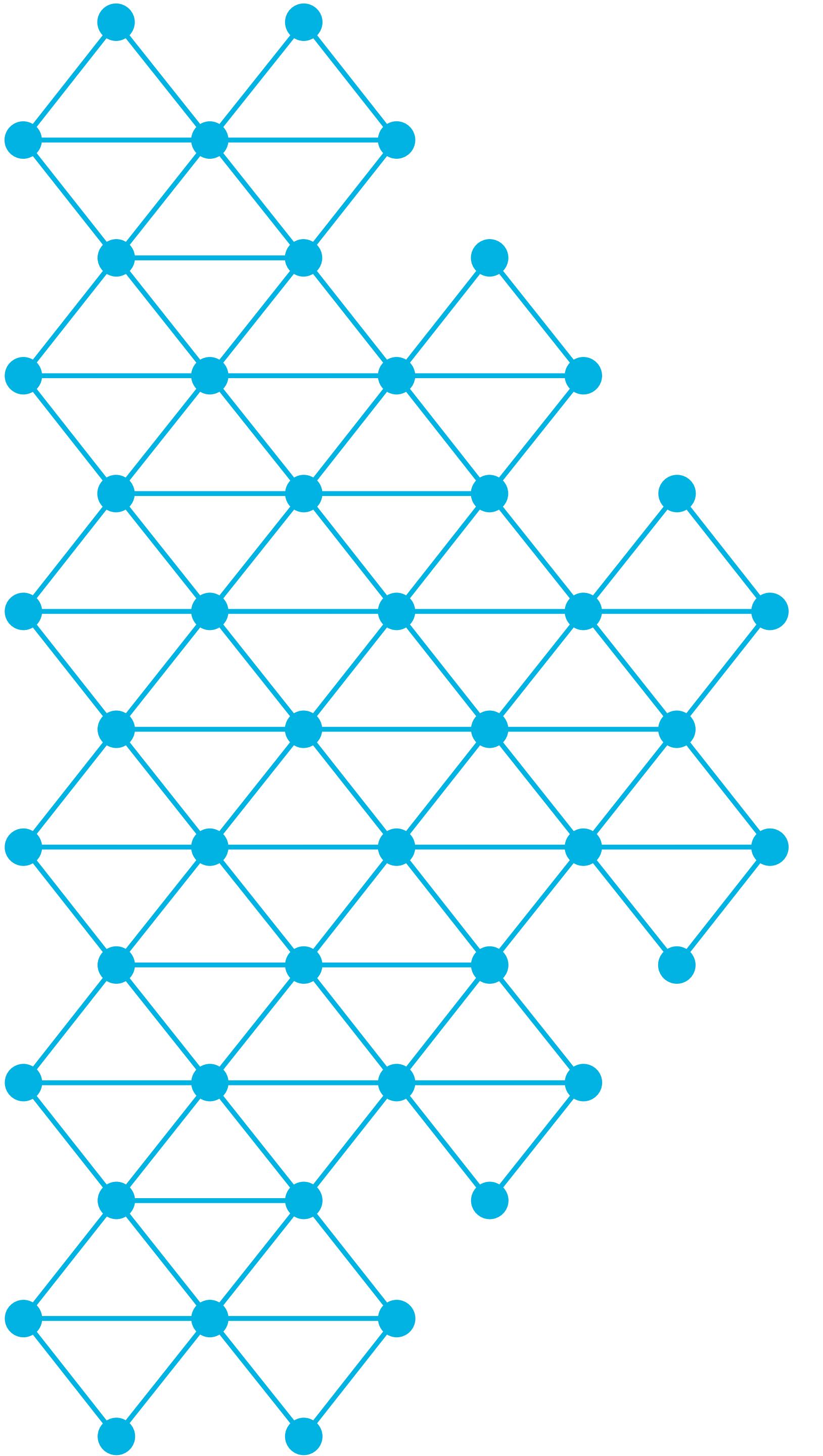
code →

$z \sim p(z); \quad x = h_\theta(z)$



# Overview

- **Background**
  - Recap: MLE, maximum marginal likelihood, EM
  - Approximate inference
- **Variational Inference and VAE**
  - Derivation of ELBO
  - Amortized variational inference
  - Stochastic variational inference
- **Better model assumption**
  - What's a good prior  $p(z)$ ?
  - What's a good likelihood  $p(x|z)$ ?
- **Better inference**
  - How to improve  $q(z|x)$ ?

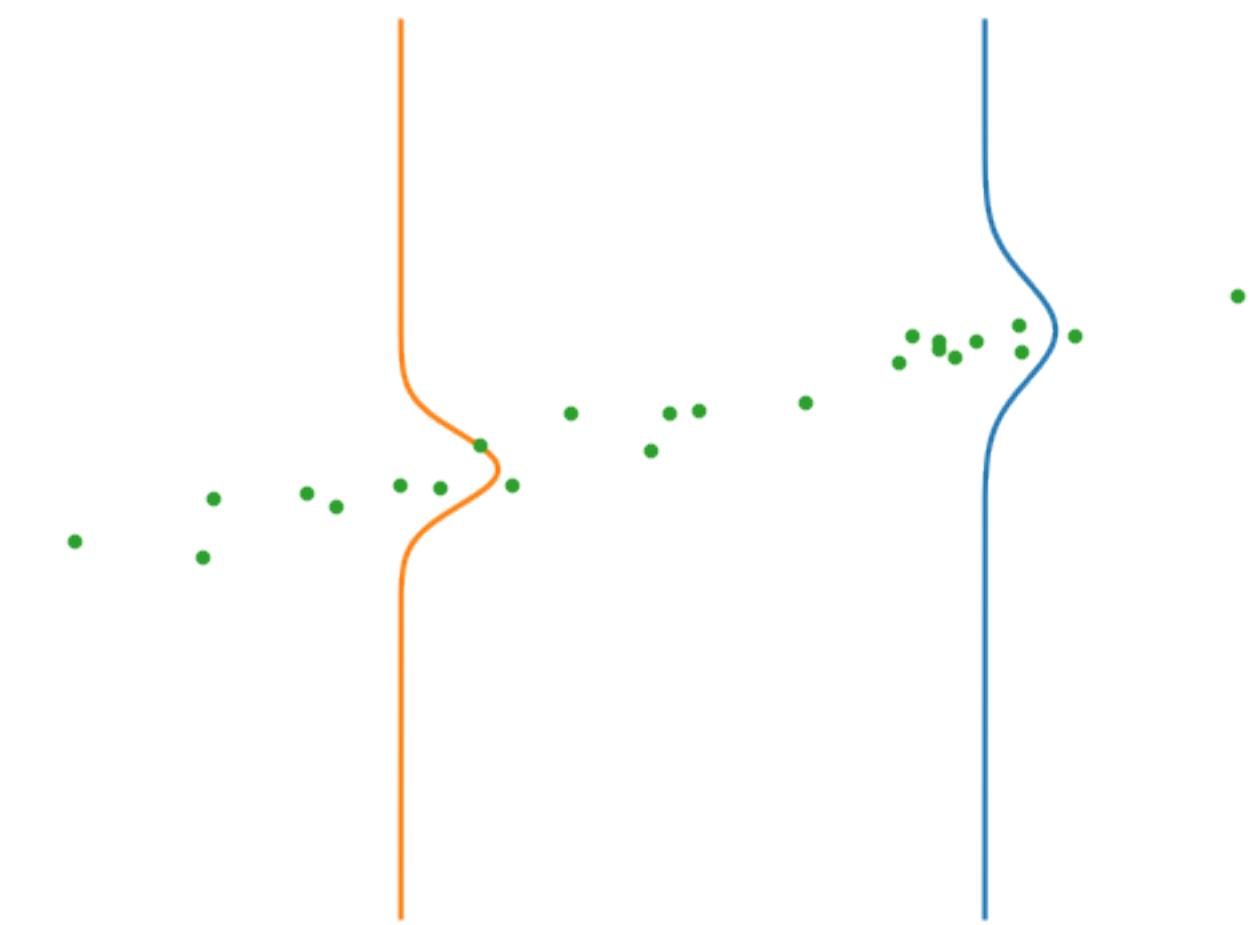
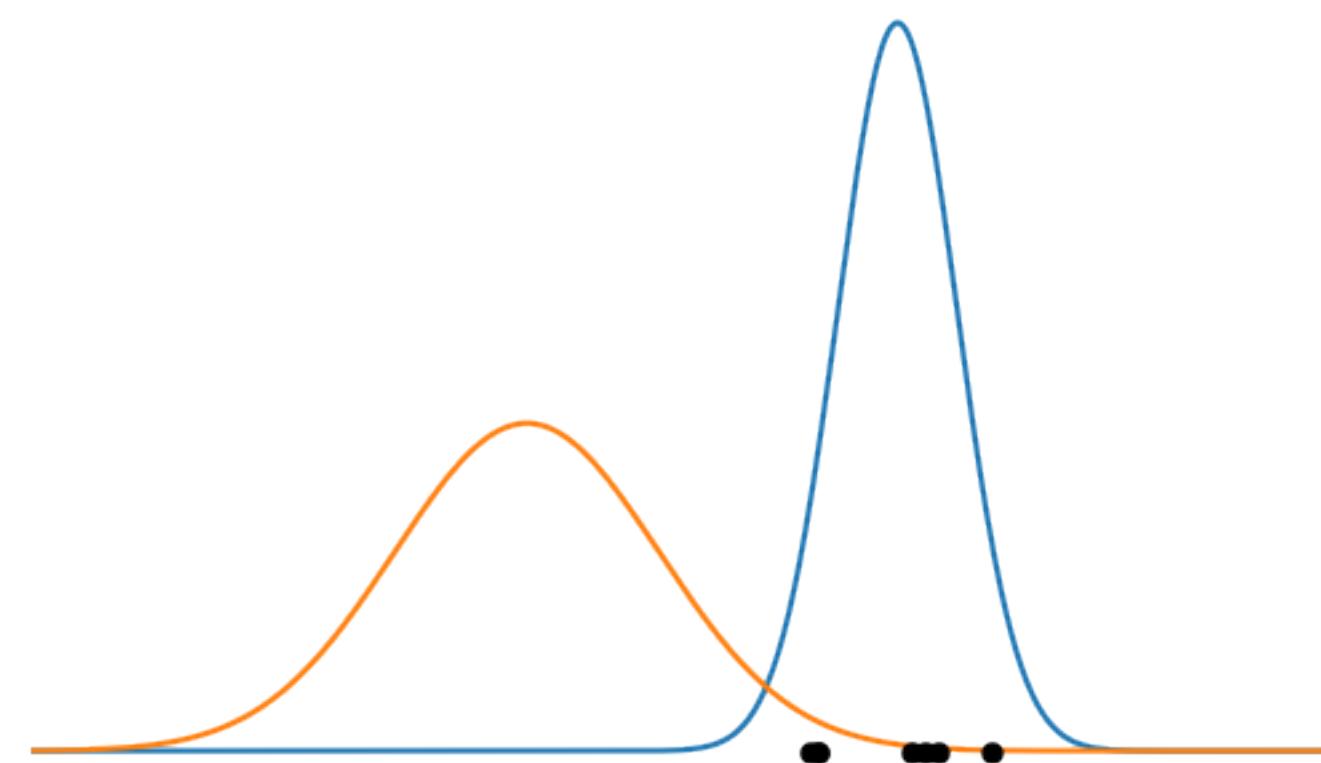


# Background

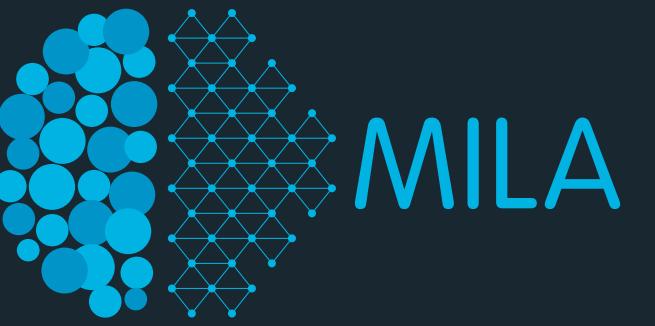
# Maximum Likelihood Recap



- **Maximum Likelihood:** Maximize the likelihood of the data being generated by your model;  $\log p(x)$
- **Maximum Conditional Likelihood:** Given pairs of data, maximize the likelihood of the target data following the mapping defined by your model;  $\log p(y|x)$



# Training Latent Variable Models



- **Maximum Marginal Likelihood:** In the face of incomplete data, maximize the observed data's likelihood governed by the marginal distribution;

$$\log p(x) = \log \int_{\lambda \in \Lambda} p(x, \lambda) d\lambda$$

- Gradient descent-based methods work for some discrete cases, when the latent variable is enumerable:

$$\log p(x) = \log \sum_{z \in Z} p(x, z) = \log \sum_{z \in Z} p(x|z)p(z)$$

# Expectation-Maximization

- EM is a coordinate ascent method that maximizes the following objective, known as the **Evidence Lower Bound** (ELBO):

$$\mathcal{L}(\theta, \phi) = \underbrace{\mathbb{E}_{z \sim q_\phi(z)} [\log p_\theta(x, z)]}_{\text{Expected complete data likelihood}} + \underbrace{\mathcal{H}(q_\phi(z))}_{\text{Entropy}}$$

E step:

$$q_{t+1} \leftarrow \operatorname{argmax}_q \mathcal{L}(p_t, q) = p_t(z|x)$$

M step:

$$p_{t+1} \leftarrow \operatorname{argmax}_p \mathcal{L}(p, q_{t+1})$$

- What is Bayes Rule? What is the prior and posterior probability?

# Approximate Inference

The need of approximate inference

$$\mathbb{E}_{z \sim q_\phi(z)} [\log p_\theta(x, z)]$$

make a guess!

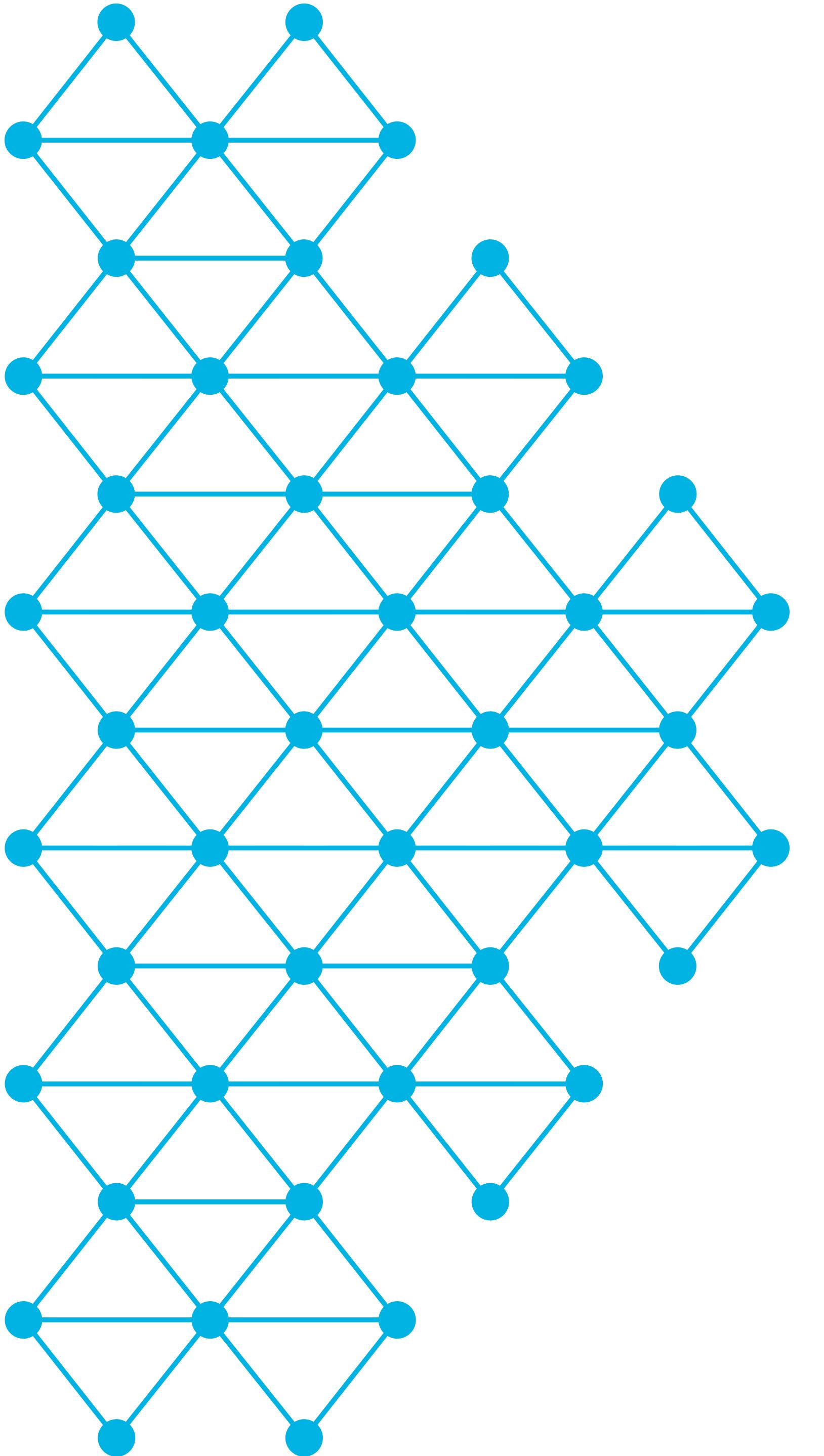
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## Markov Chain Monte Carlo

- Sampling method
- Unbiased but high variance

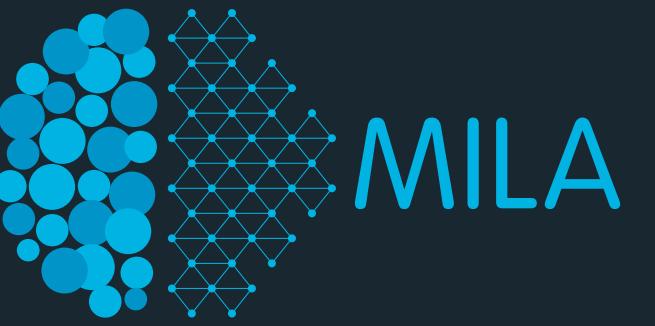
## Variational Inference

- Optimization method
- **Low variance** but biased



# Variational Inference and VAE

# Evidence Lower BOund (ELBO)



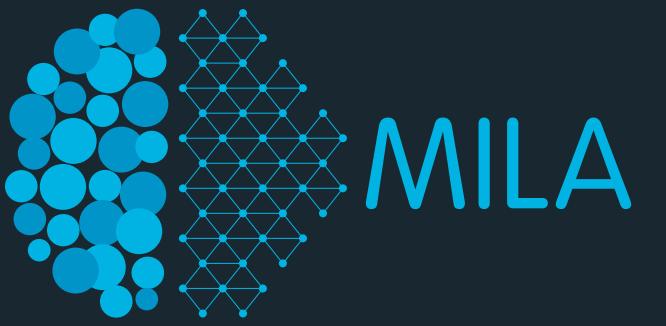
- Define the joint probability as  $p(x,z) = p(x|z)p(z)$ 
    - 1.  $z \sim p(z)$ ; e.g.  $p(z) = \mathcal{N}(z; 0, I)$
    - 2.  $x \sim p(x|z) = p(x; \text{dec}(z))$ ; e.g.  $p(x|z) = \text{Bern}(x; \pi(z))$
- .....

# Variational Gap

$$\begin{aligned}
 \log p(x) - \overbrace{\mathbb{E}_{z \sim q(z)} [\log p(x, z) - \log q(z)]}^{\mathcal{L}(p, q)} \\
 &= \mathbb{E}_{z \sim q(z)} [\log q(z) - \log \frac{p(x, z)}{p(x)}] \\
 &= \mathbb{E}_{z \sim q(z)} [\log q(z) - \log p(z|x)] \\
 &= D_{\text{KL}} (q(z) \| p(z|x))
 \end{aligned}$$

$\log p(x)$      $\xrightarrow{\hspace{1cm}}$   
 $\downarrow$                   *Approximation Gap*  
 $\mathcal{L}[q^*]$      $\xleftarrow{\hspace{1cm}}$

# Amortized Variational Inference



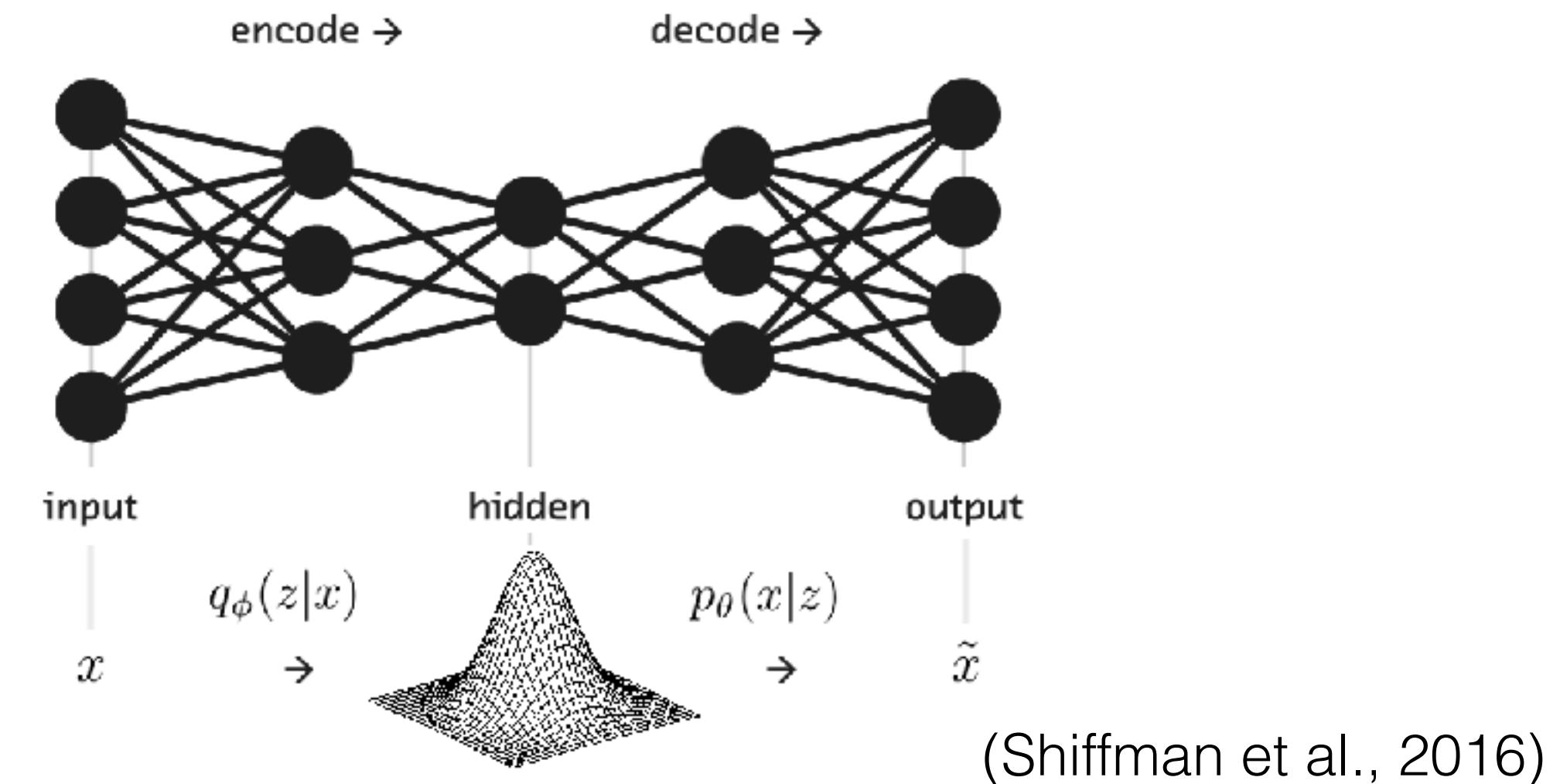
## Traditional VI

- For each data instance  $x_i$  there is a variational approximation  $q_i$
- When the true posterior  $p(z|x_i)$  is not tractable, we need to keep track of the  $q_i$  for each  $i$

## Amortized VI

- Use an **inference network** (encoder)  $q_\phi(z|x_i)$

$$\begin{aligned}\mathcal{L}_i(\theta, \phi) &= \mathbb{E}_{z \sim q_\phi(z|x_i)} [\log p_\theta(x_i, z) - \log q_\phi(z|x_i)] \\ &= \underbrace{\mathbb{E}_{z \sim q_\phi(z|x_i)} [\log p_\theta(x_i|z)]}_{\text{reconstruction term}} - \underbrace{D_{\text{KL}} (\log q_\phi(z|x_i) \| p(z))}_{\text{regularization term}}\end{aligned}$$

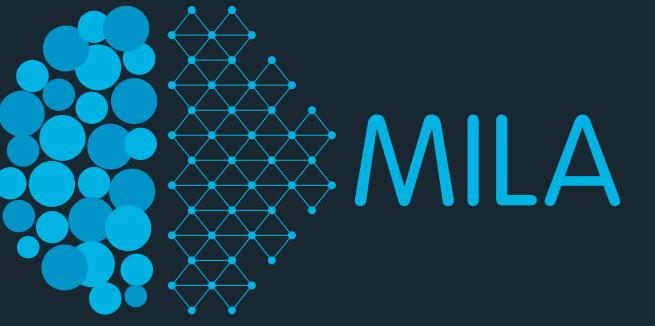


Amortized inference (Gershman & Goodman, 2014)

Auto-encoding variational bayes, AEVB (Kingma & Welling, 2014)

Recognition model (Rezende et al, 2014)

# Stochastic Variational Inference



- We want to estimate the gradient of the ELBO (Monte Carlo)

$$\begin{aligned}\nabla \mathcal{L}_i &= \mathbb{E}_z [(\log p(x_i, z) - \log q(z|x_i)) \nabla \log q(z|x_i)] \\ &\approx \frac{1}{M} \sum_{m=1}^M (\log p(x_i, z_m) - \log q(z_m|x_i)) \nabla \log q(z_m|x_i) \quad z_m \sim q(z|x_i)\end{aligned}$$

unbiased, high variance

Remedies:

More samples  
Rao-Blackwellization  
Control Variate  
Baseline ...

Other gradient estimator?

# Reparameterization Trick

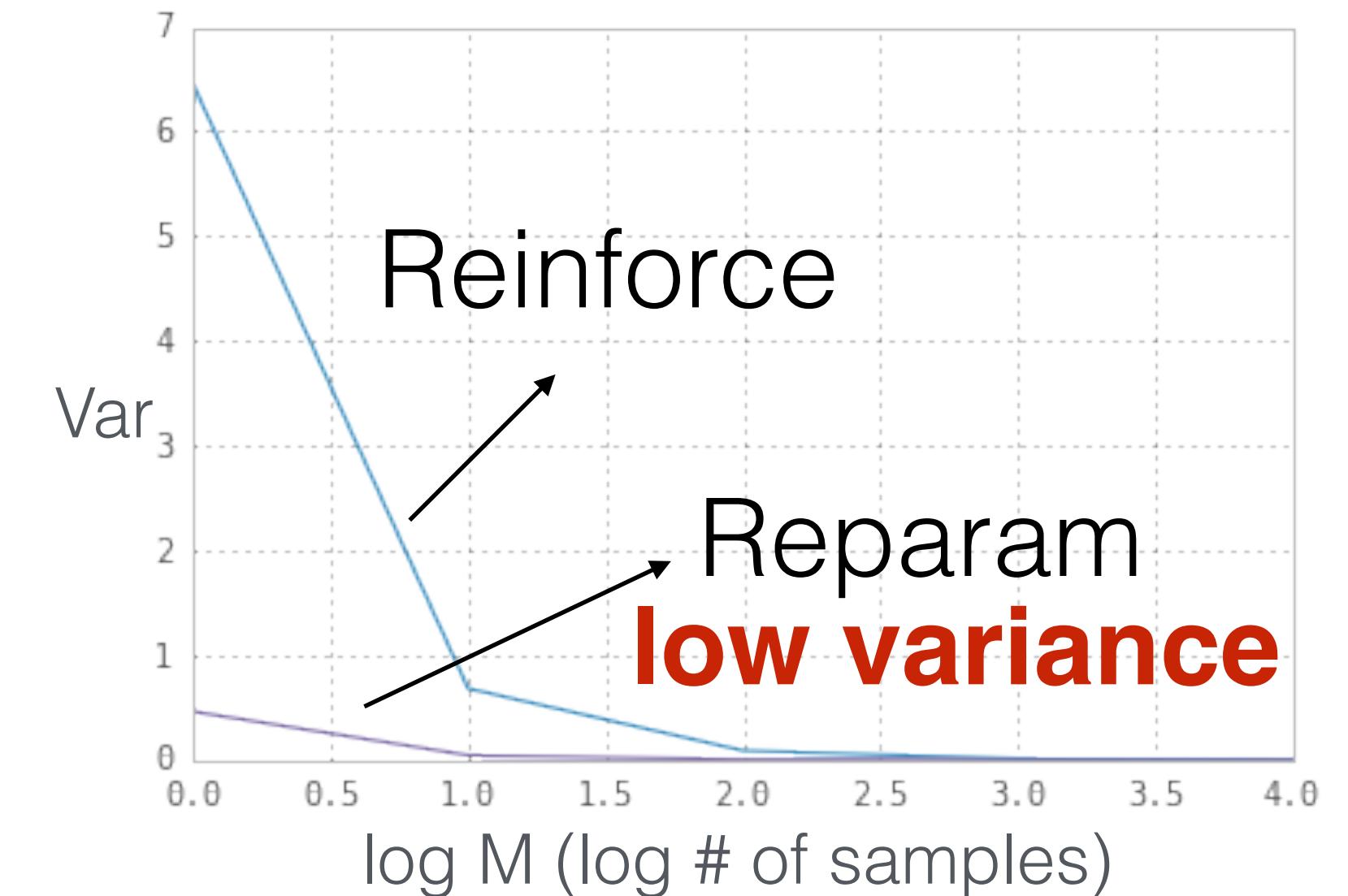
- Decompose the sampling process into

$$z \sim q_\phi(z|x) \Leftrightarrow \epsilon \sim q(\epsilon);$$

$$z = g_\phi(\epsilon, x)$$

$$z \sim \mathcal{N}(z; \mu_\phi(x), \sigma_\phi^2(x)) \Leftrightarrow \epsilon \sim \mathcal{N}(\epsilon; 0, I);$$

$$z = \sigma(x) \odot \epsilon + \mu(x)$$



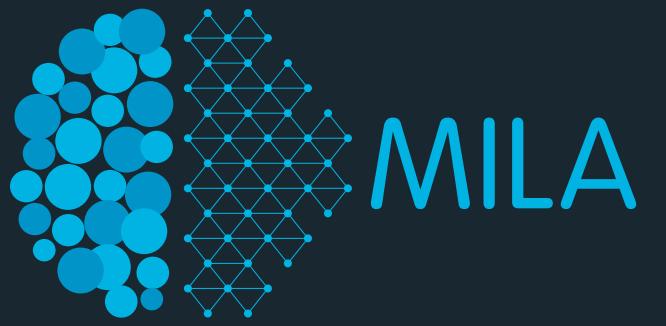
*How to estimate the gradient then?*

Doubly Stochastic Variational Bayes (Titsias & Lazaro-Gredilla, 2014)

Stochastic Gradient Variational Bayes, SGVB (Kingma & Welling, 2014)

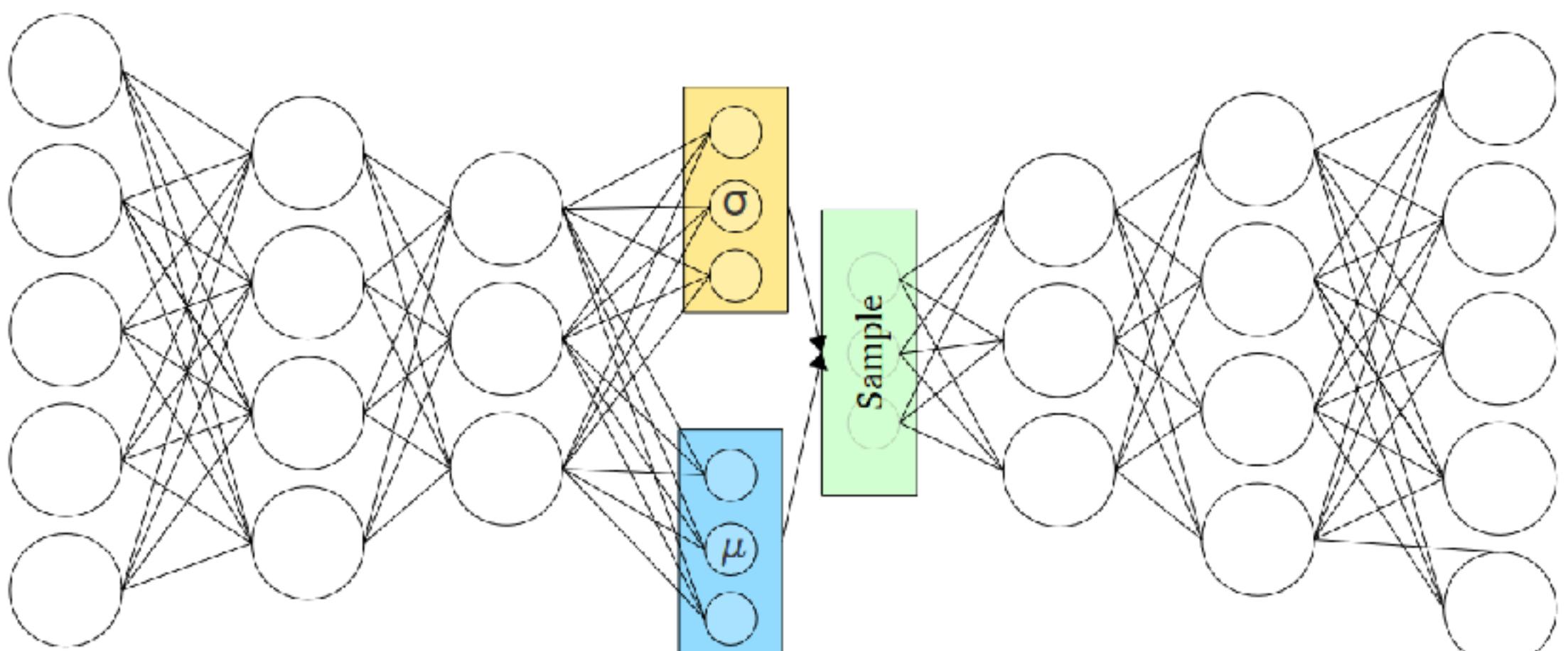
Stochastic Backpropagation (Rezende et al, 2014)

# Variational Auto-Encoder (VAE)

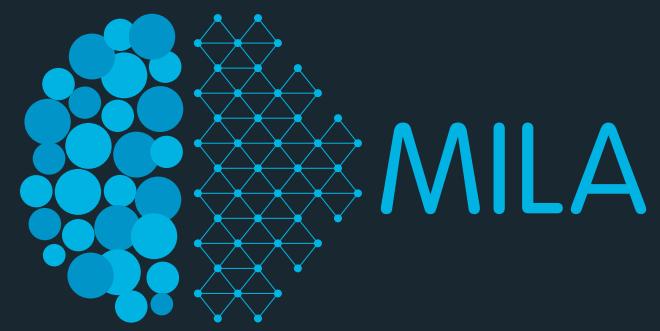


- Vanilla VAE

$$p(z) = \mathcal{N}(0, \mathbf{I}); \quad p(x|z) = \prod_j p(x_j|z); \quad q(z|x) = N(\mu(x), \text{diag}(\sigma^2(x)))$$



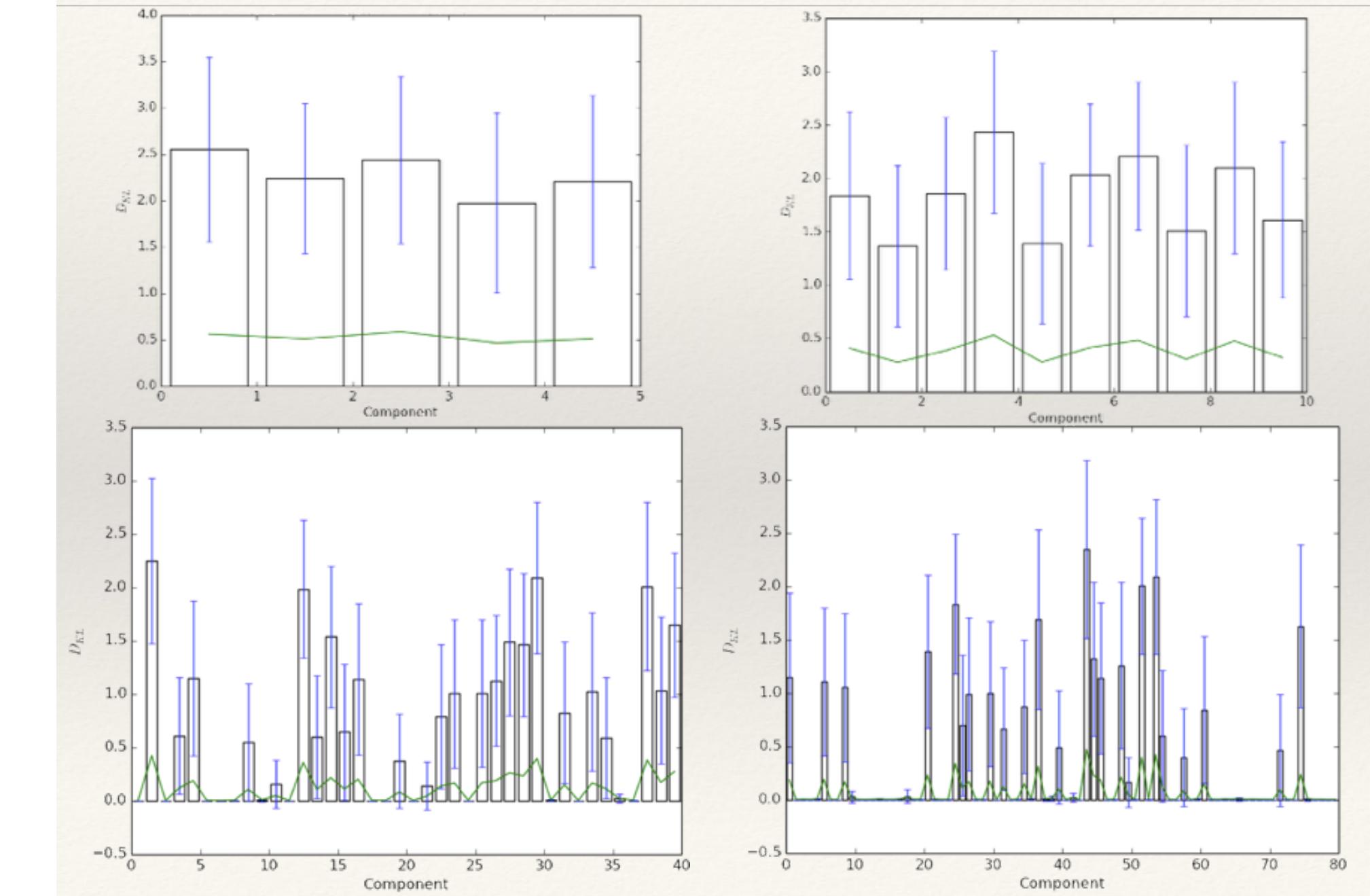
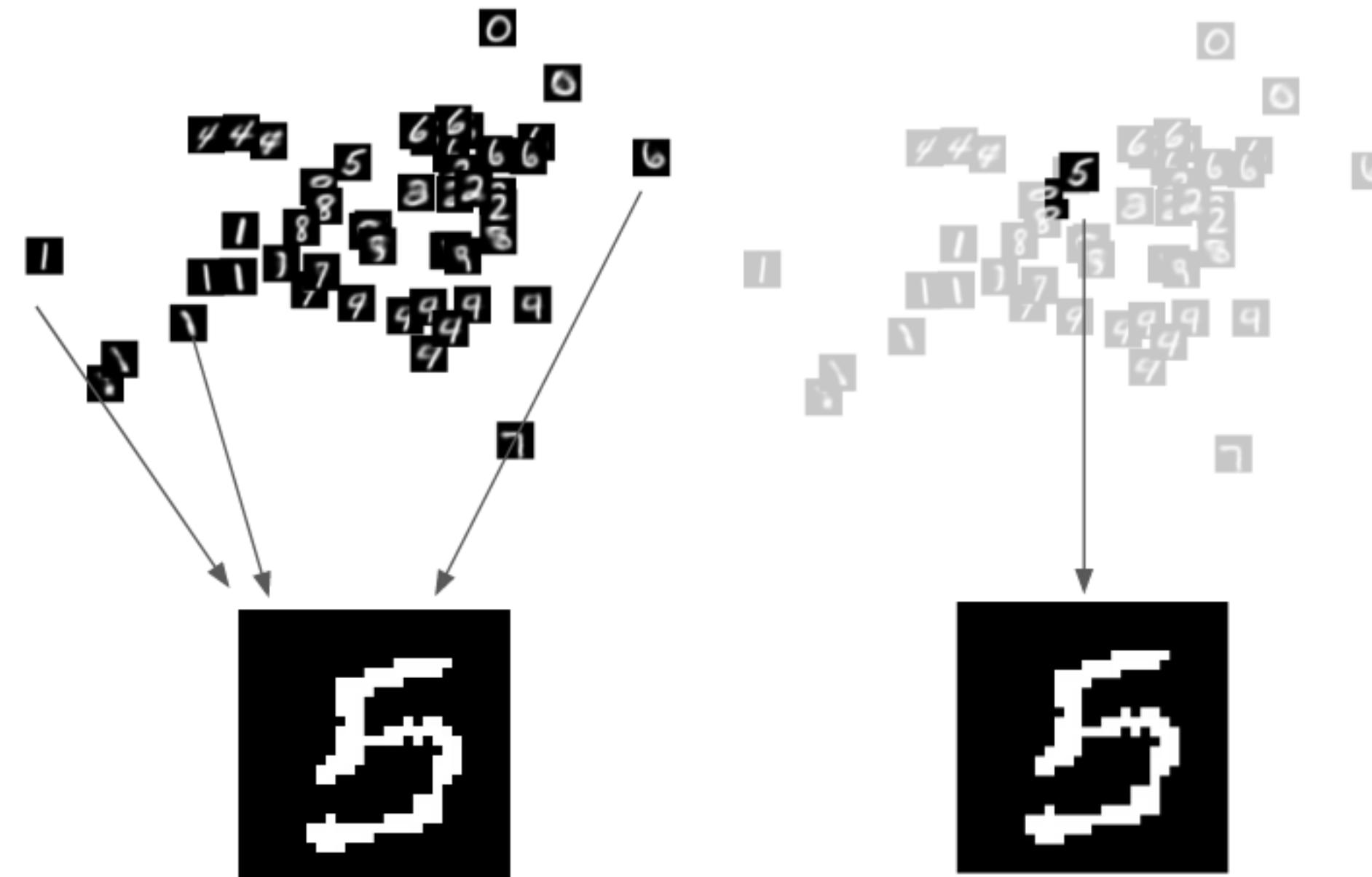
# Caveats, Information Theoretic POV



- Regularized Autoencoder?

the smaller the better?

$$\underbrace{\mathbb{E}_{z \sim q_\phi(z|x_i)} [\log p_\theta(x_i|z)]}_{\text{reconstruction loss}} - \underbrace{D_{\text{KL}} (\log q_\phi(z|x_i) \| p(z))}_{\text{regularization term}}$$



# Evaluation

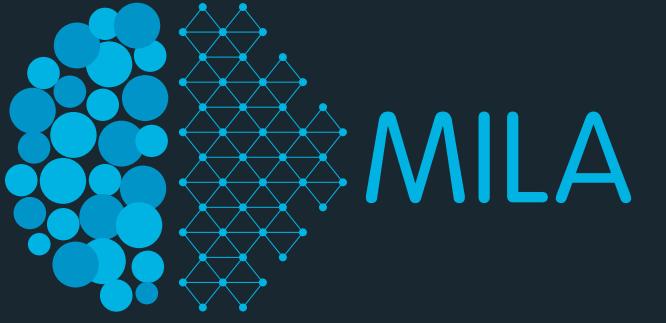
- Importance Sampling (stochastic lower bound)

$$p(x) \approx \frac{1}{M} \sum_{m=1}^M \frac{p(x, z_m)}{q(z_m | x)}$$

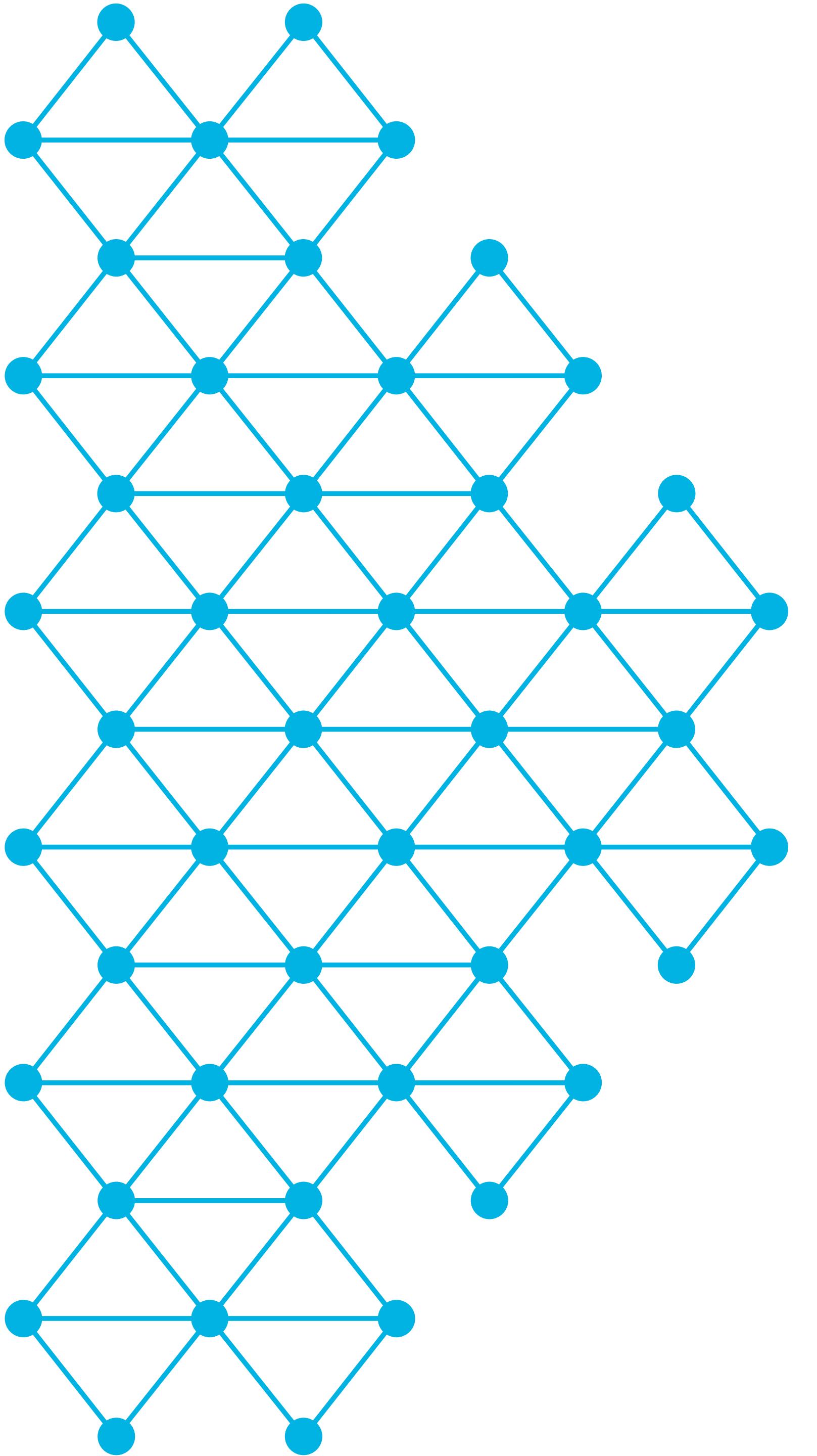
$$\log p(x) \approx \text{L}\Sigma\text{E}_{m=1}^M [\log p(x, z_m) - \log q(z_m | x)]$$

- Further reading: Annealed Importance Sampling by Radford Neal

# What Assumptions have we made so far?

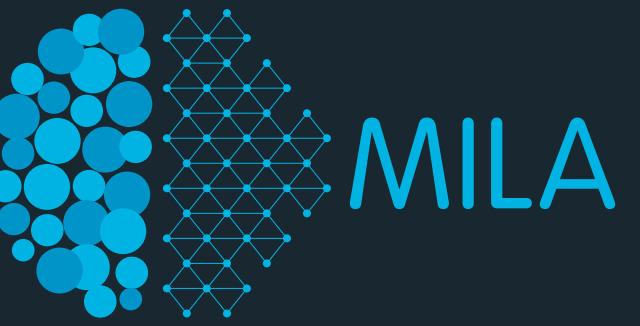


- What can we change? (Non-Vanilla VAE)
  - fixing  $p(z) = \mathcal{N}(0, \mathbf{I})$
  - fixing  $p_{\theta}(x|z) = \prod_j p_{\theta}(x_j|z); \quad \Theta : \theta \in \Theta$
  - fixing  $\mathcal{Q} : q \in \mathcal{Q}$
  - using  $q_{\phi}(z|x_i)$  instead of  $q_i(z)$  ; fixing  $\Phi : \phi \in \Phi$



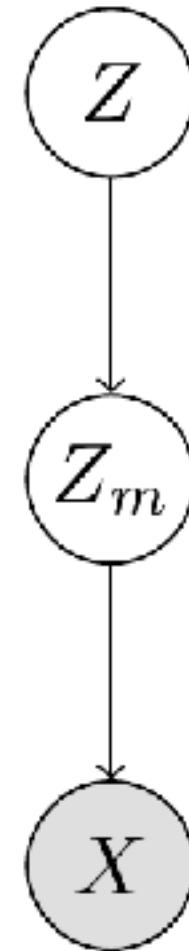
# Better Model Assumptions

# What likelihood $p(x|z)$ to use?



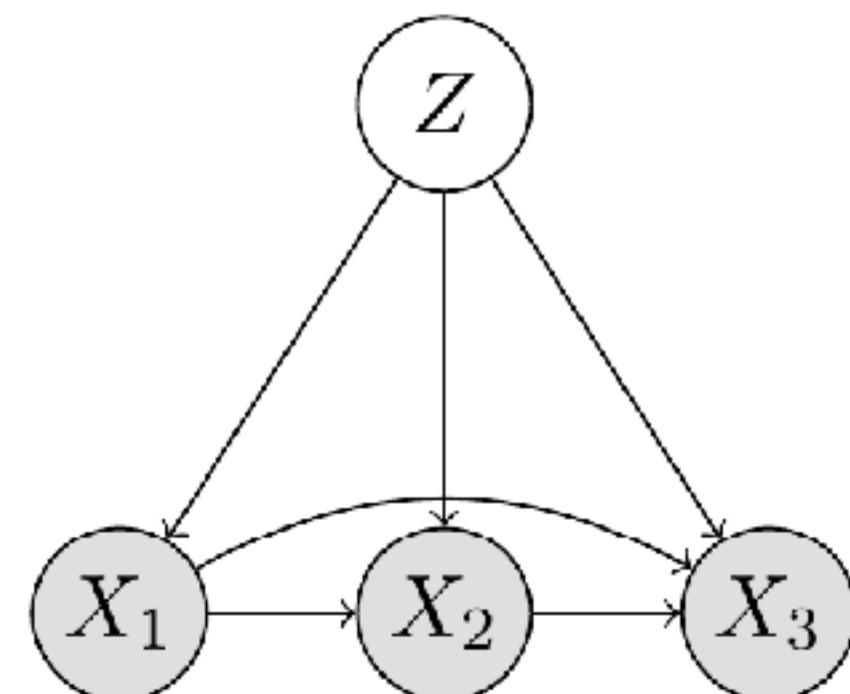
- Hierarchy?

$$p(x|z) = \int_{z_{mid}} p(x, z_{mid}|z) dz_{mid}$$

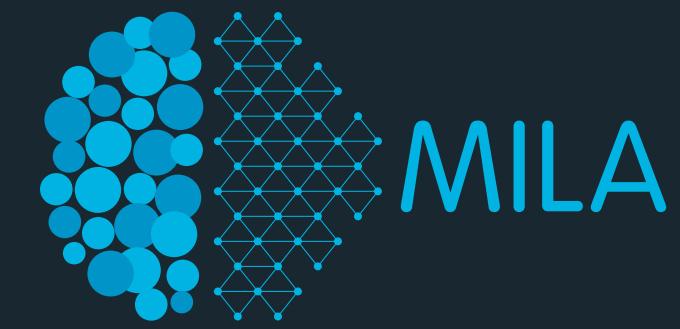


- Autoregressive model?

$$p(x|z) = \prod_j p(x_j|x_{j'<j}, z)$$



# PixelVAE

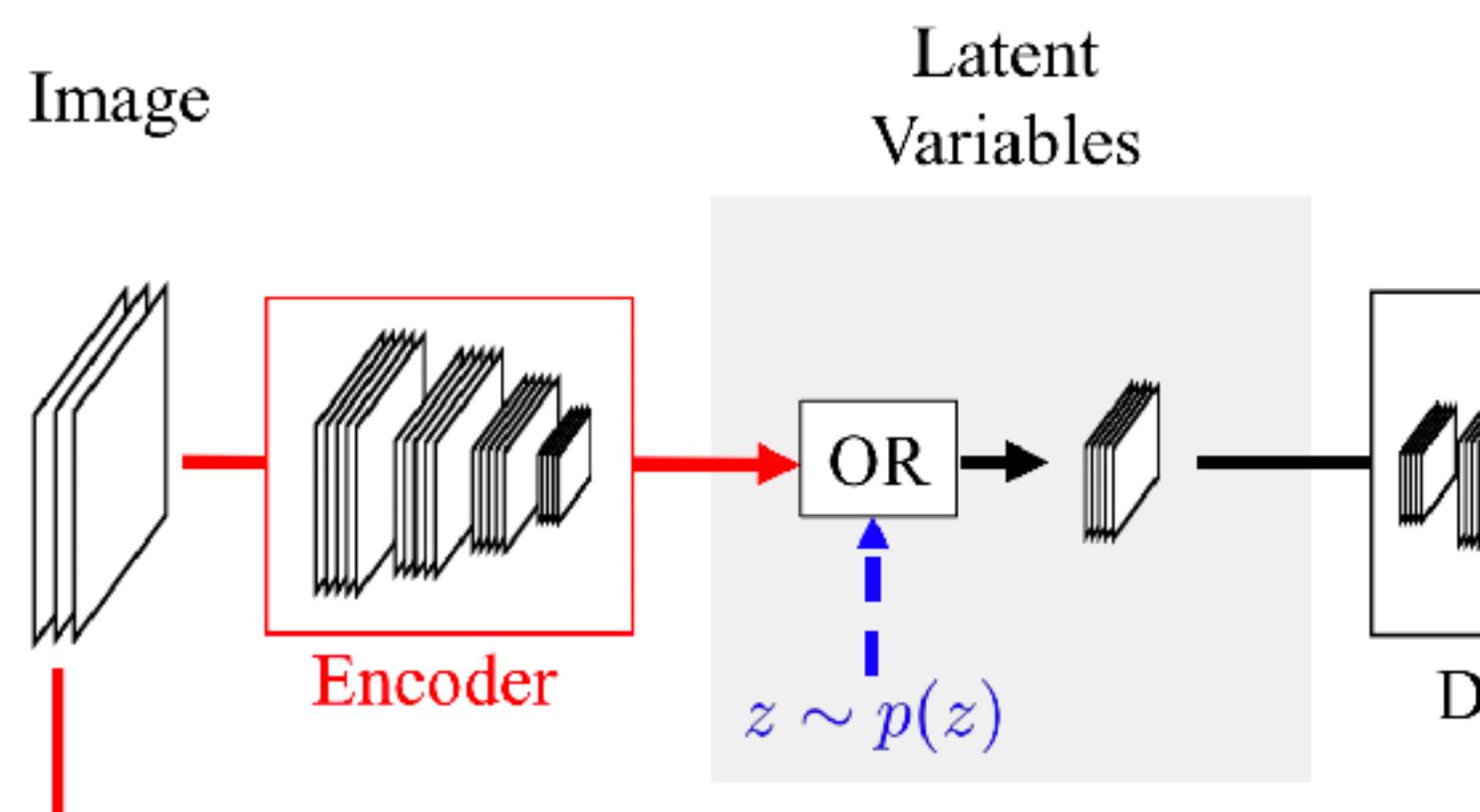
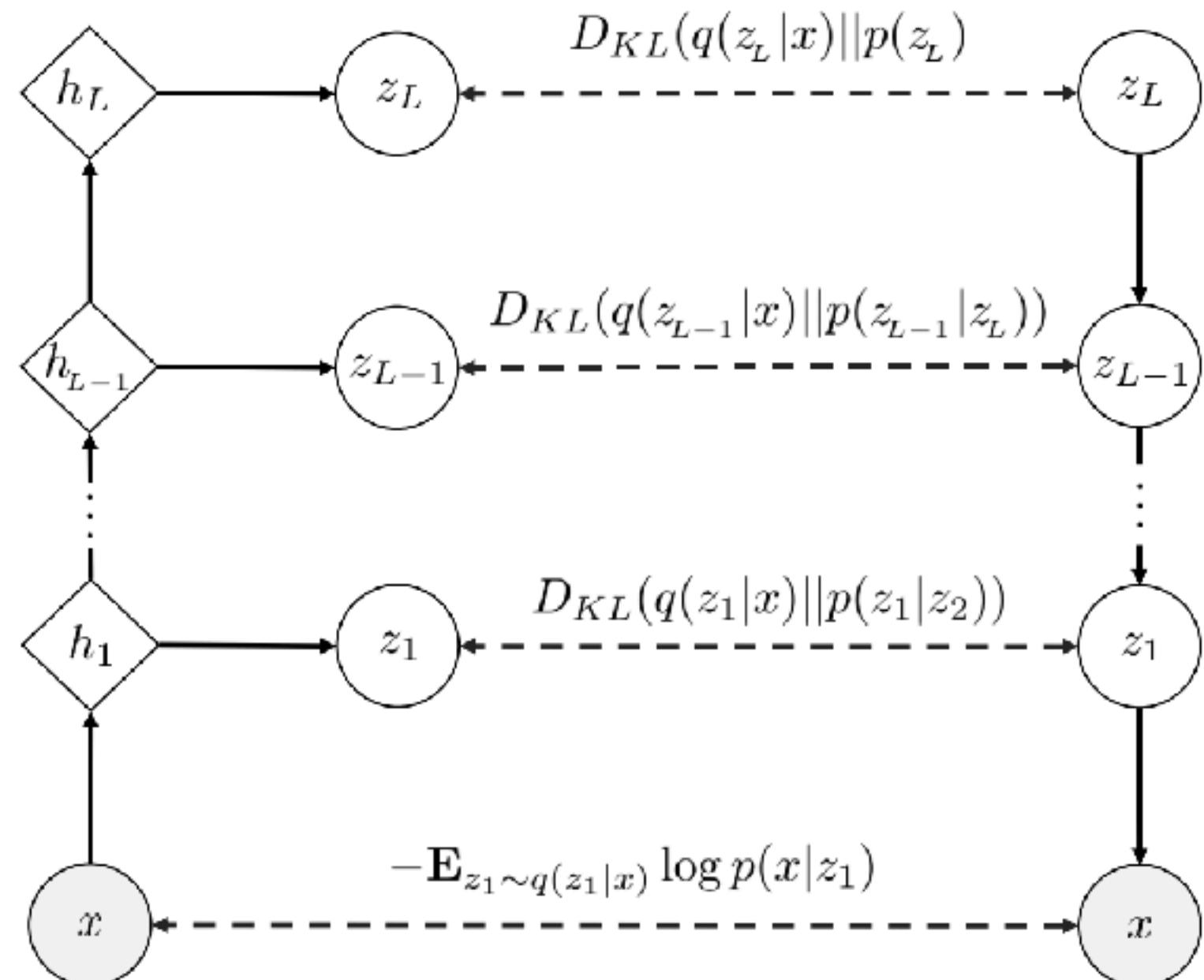


$$-L(x, q, p) = -E_{z_1 \sim q(z_1|x)} \log p(x|z_1) + D_{KL}(q(z_1, \dots, z_L|x)||p(z_1, \dots, z_L))$$

⋮

$$= -E_{z_1 \sim q(z_1|x)} \log p(x|z_1) + \sum_{i=1}^L \mathbf{E}_{z_{i+1} \sim q(z_{i+1}|x)} [D_{KL}(q(z_i|x)||p(z_i|z_{i+1}))]$$

$$p(x|z_1) = \prod_j p(x_j|x_{j'<j}, z_1)$$

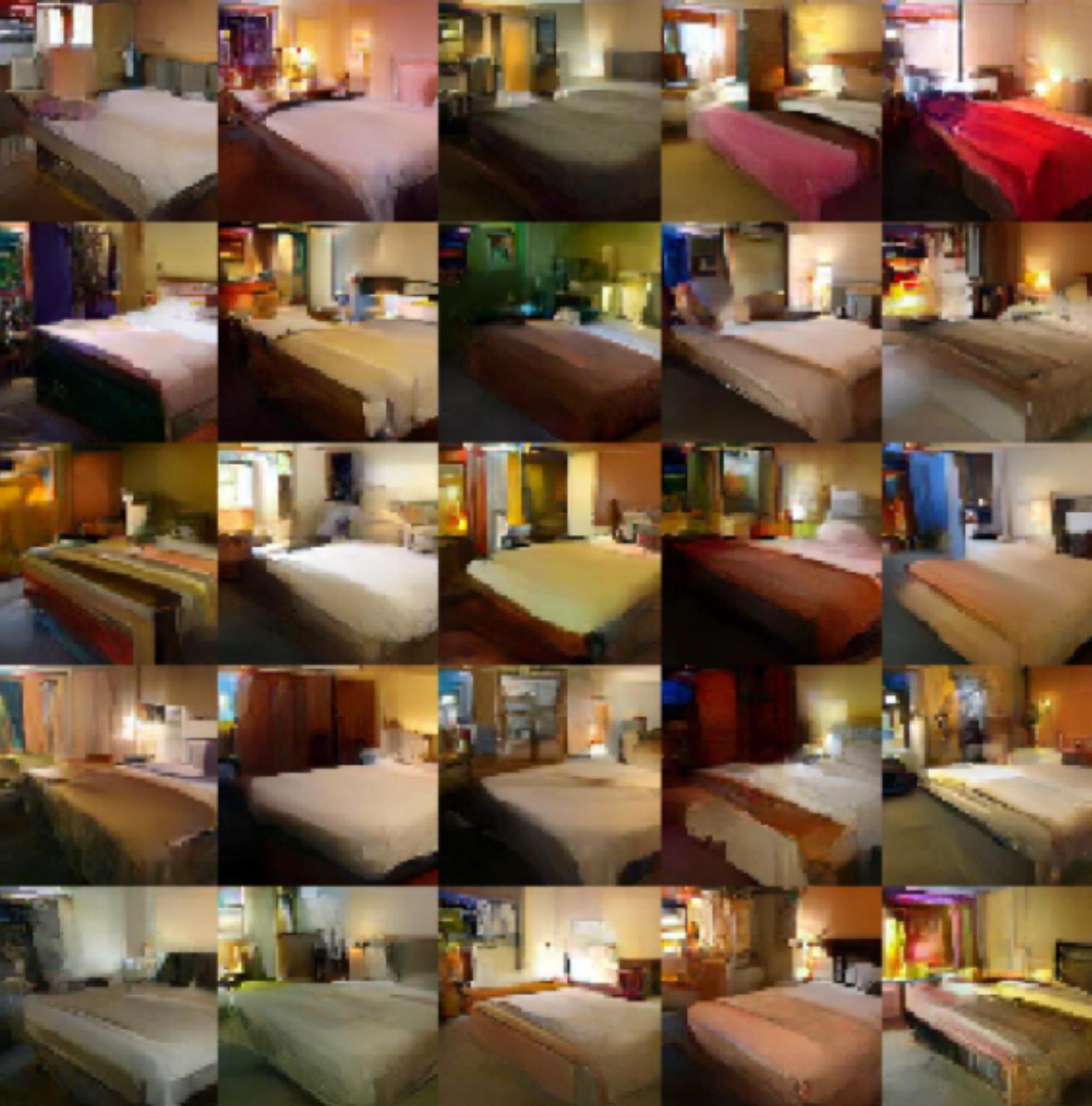


Training: Teacher forcing

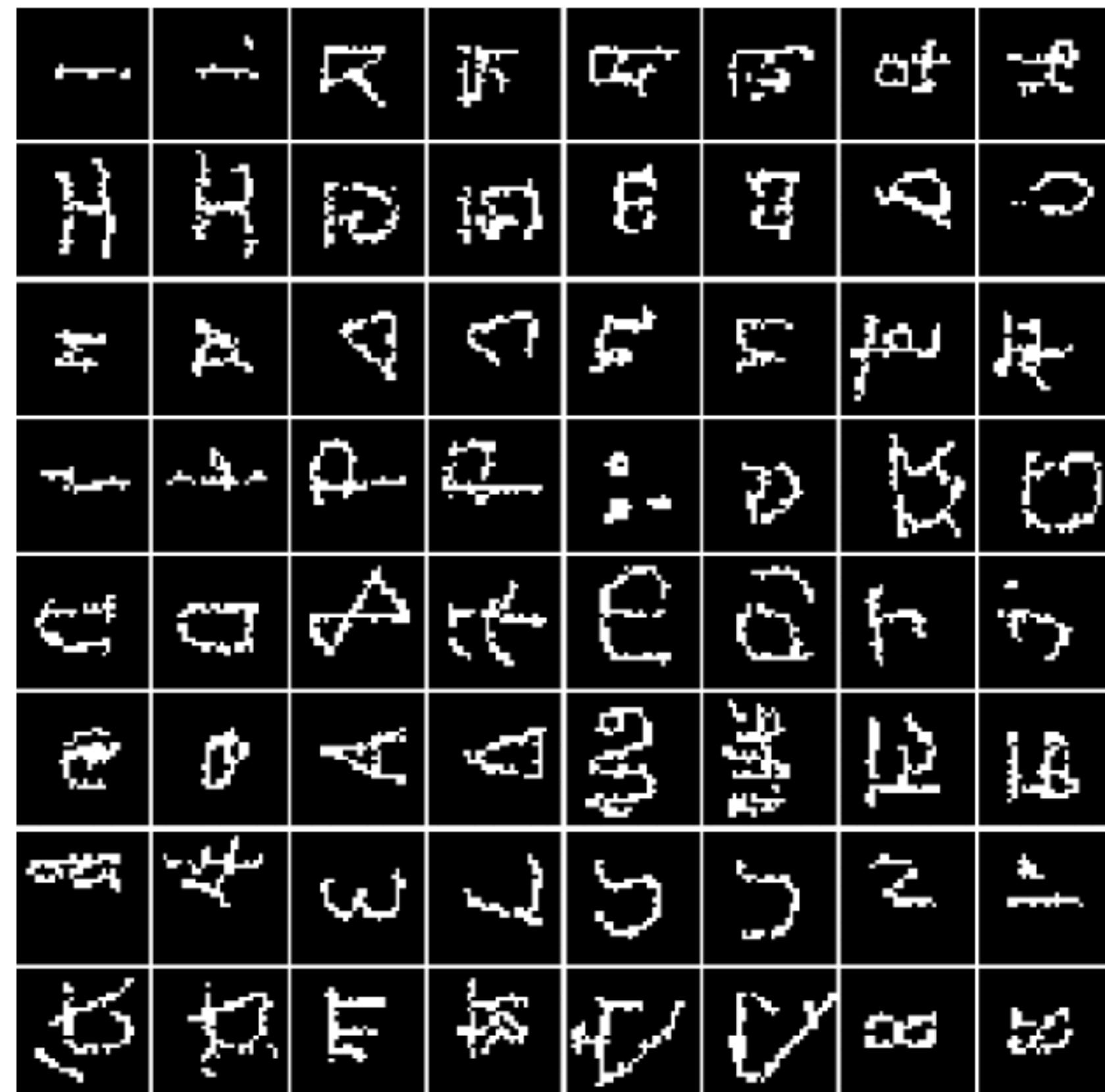
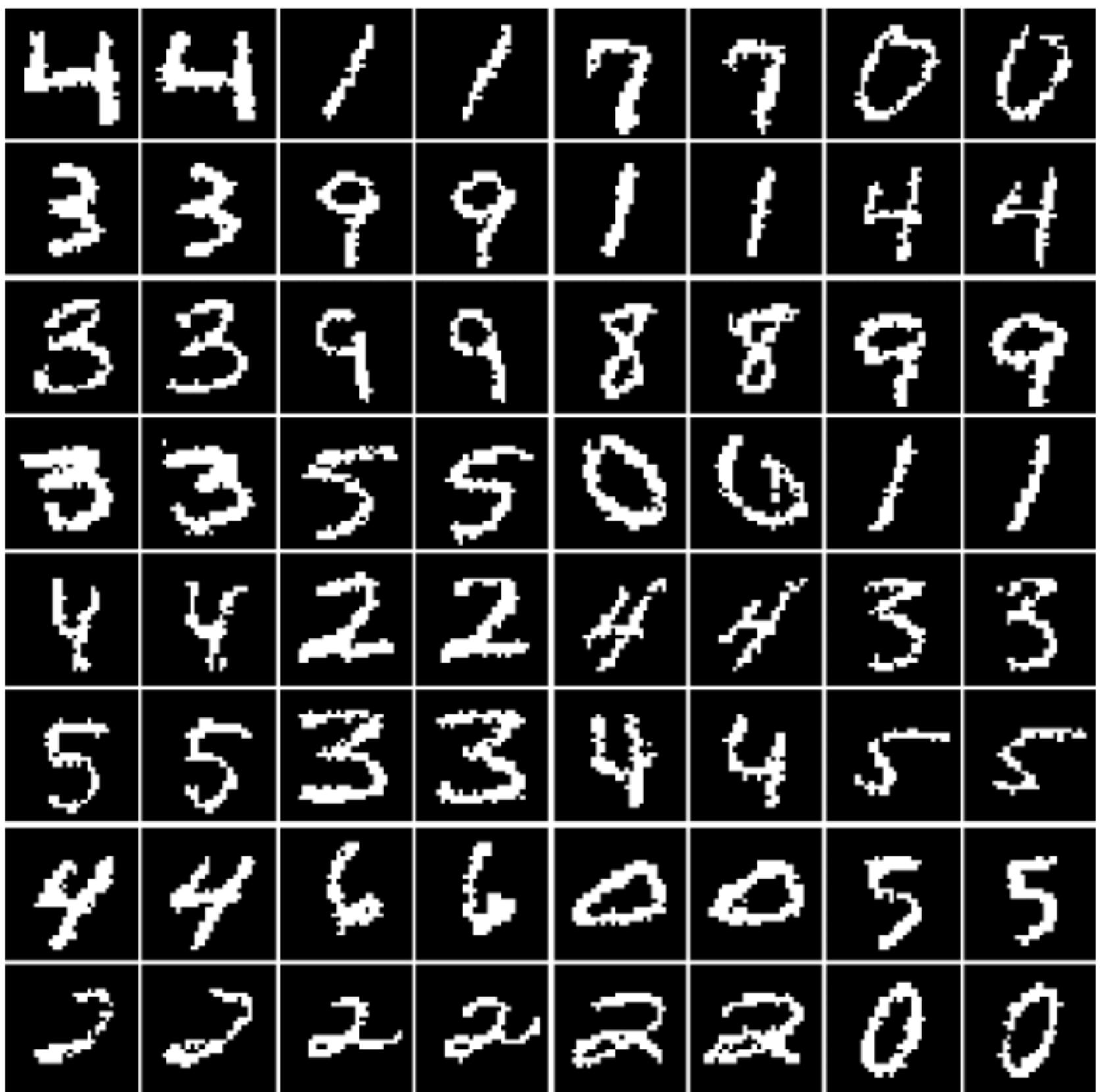
Reconstruction  
OR  
Sample

Generation:  
Autoregressive sampling

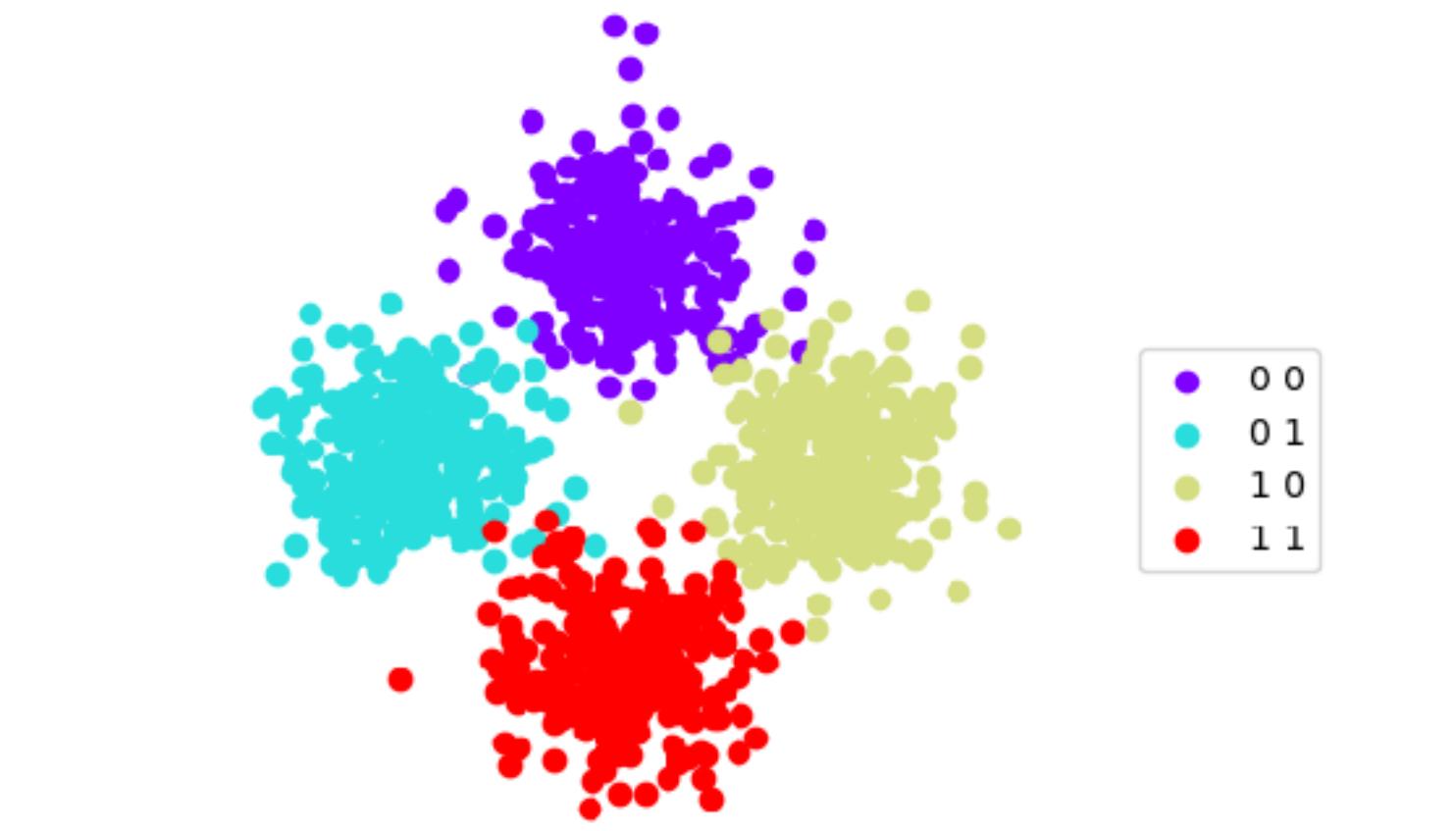
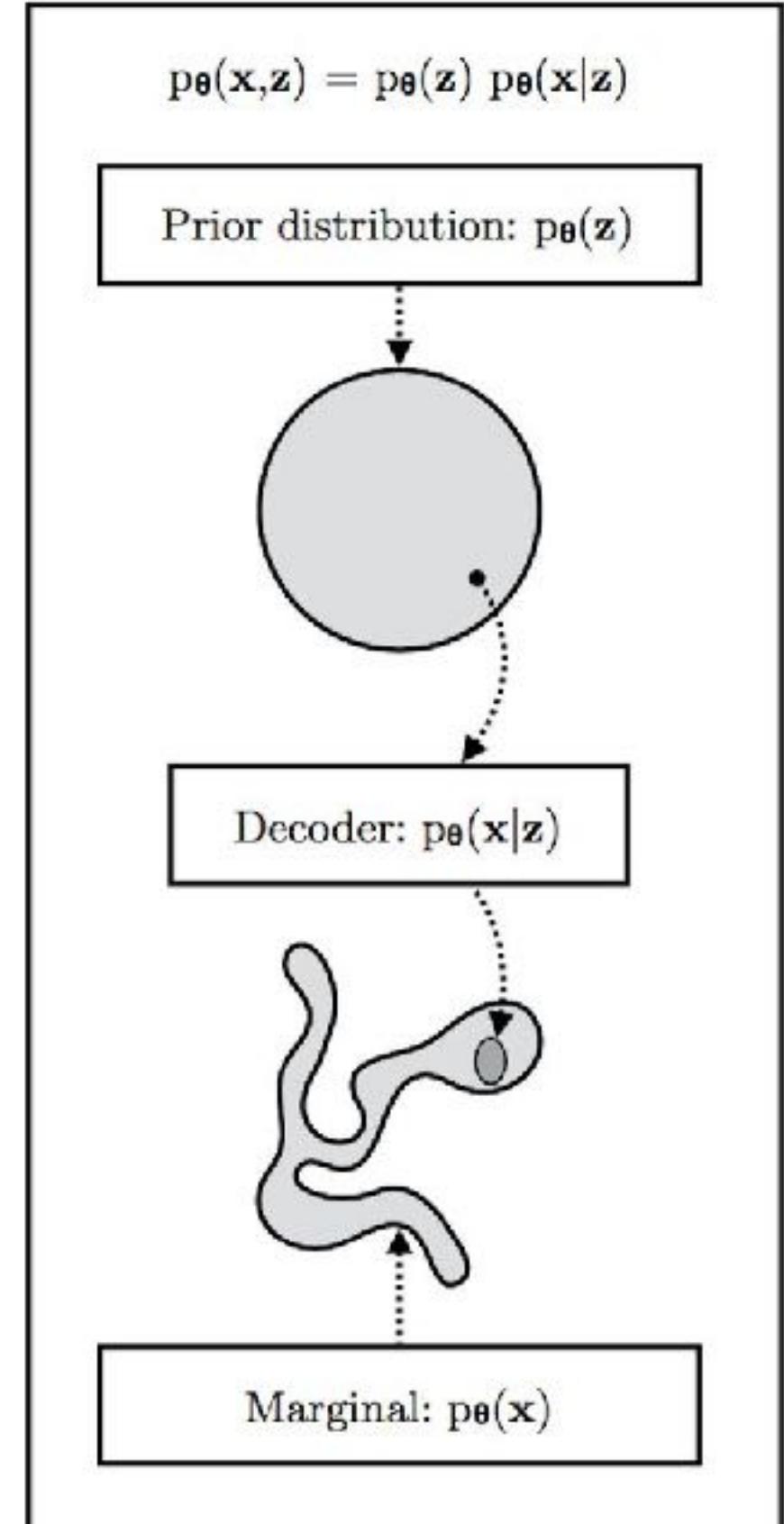
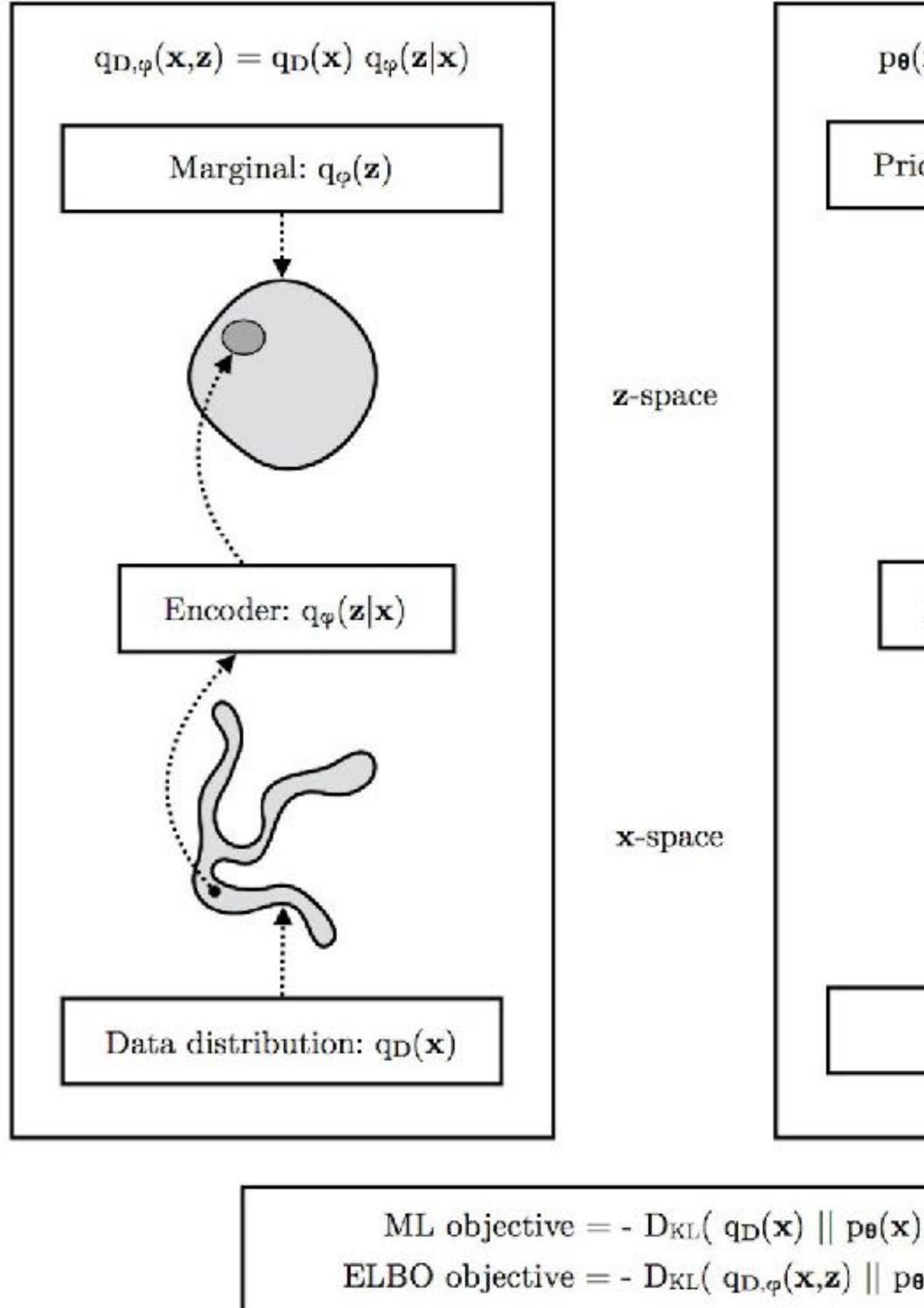
# PixelVAE samples



# Lossy Encoding

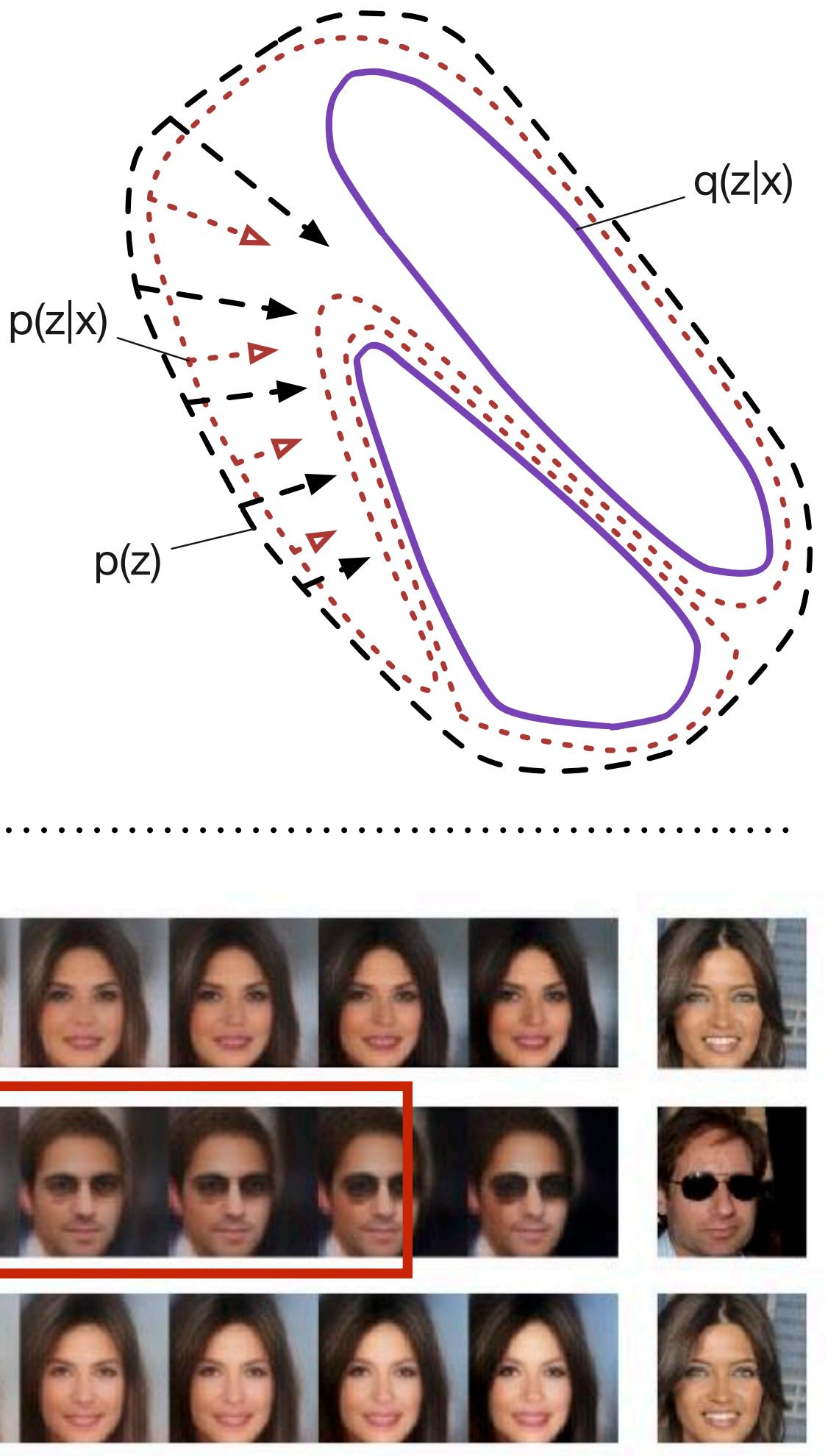


# What prior $p(z)$ to use?

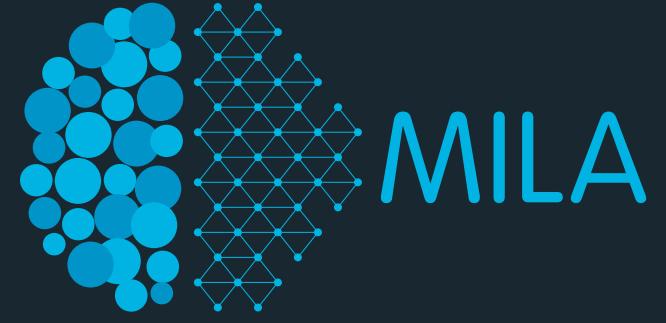


$$q(z) = \sum_x q_D(x) q_\varphi(z|x) = \mathbb{E}_{q_D(x)} [q(z|x)]$$

.....



# Prior Can Be Learned!

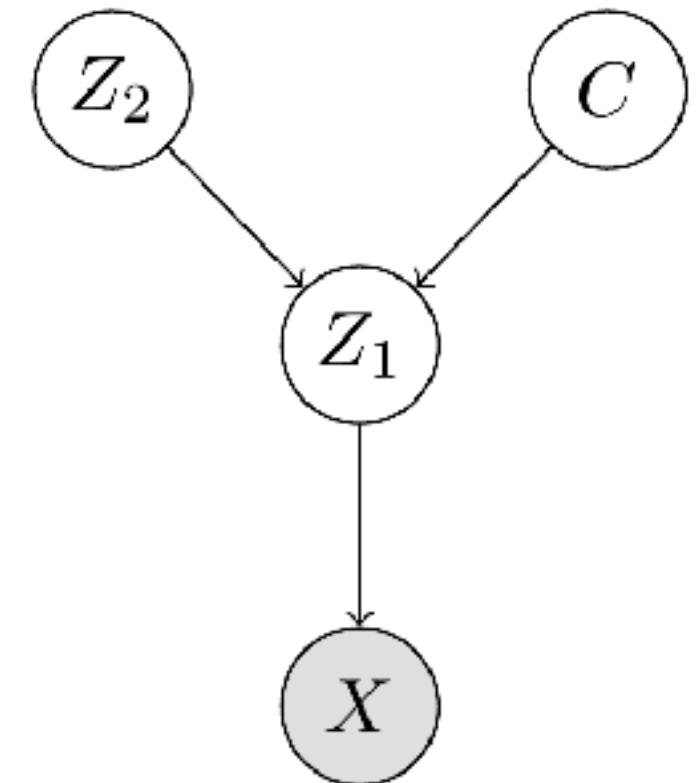


if DLGMs find it difficult to produce unimodal Gaussian marginal posteriors, then perhaps we should investigate multimodal priors that can meet  $q(z)$  halfway.

— Matt Hoffman, 2016

NIPS Workshop on Advances in Approximate Bayesian Inference Workshop

# Multimodal Prior

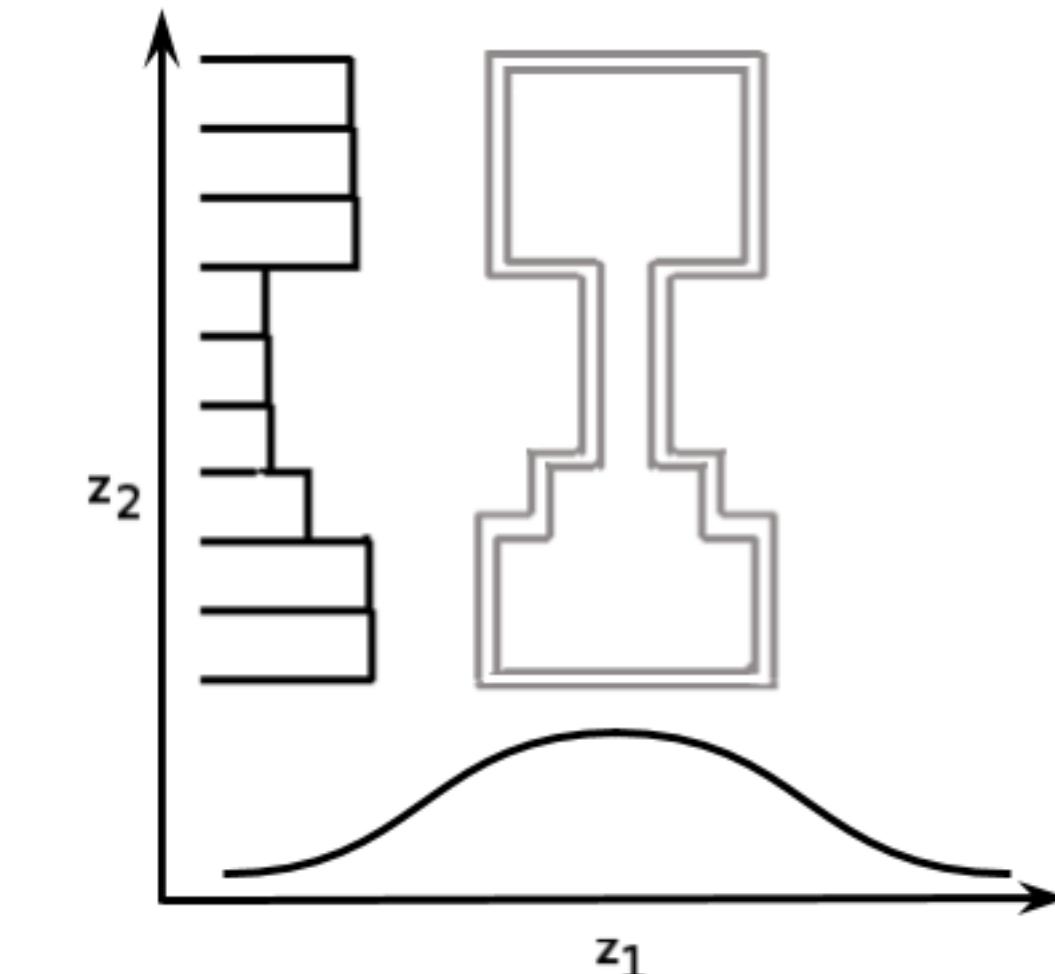


$$p(z_1|z_2) = \sum_c p(z_1|z_2, c)p(c)$$

↑  
mixture (of Gaussians) prior

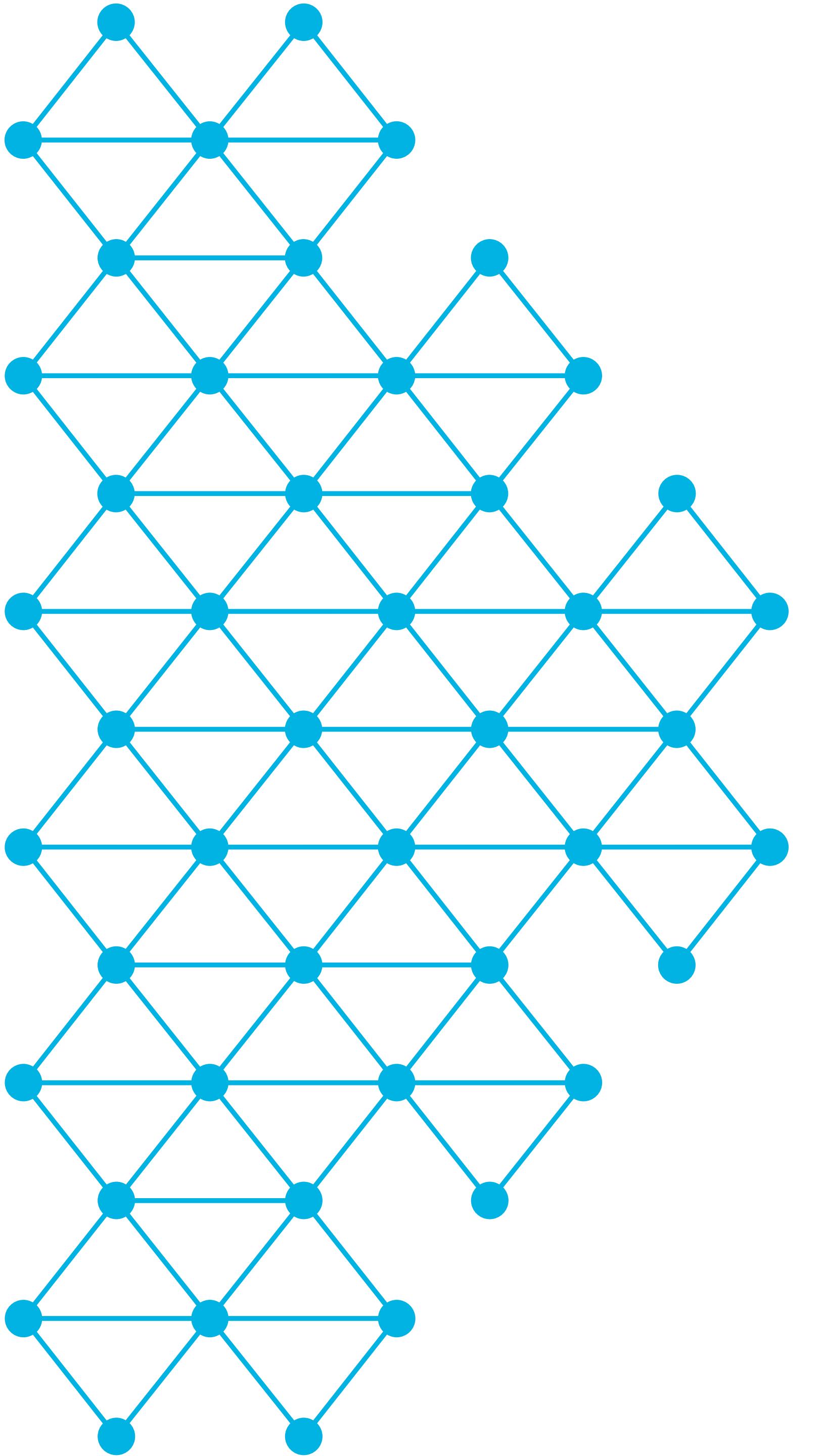
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**4 0 1 2 3 4 5 6 7 8 9**  
**9 0 1 2 3 4 5 6 7 8 9**  
**5 0 1 2 3 4 5 6 7 8 9**  
**4 0 1 2 3 4 5 6 7 8 9**  
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**7 0 1 2 3 4 5 6 7 8 9**  
**5 0 1 2 3 4 5 6 7 8 9**  
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**7 0 1 2 3 4 5 6 7 8 9**  
**1 0 1 2 3 4 5 6 7 8 9**



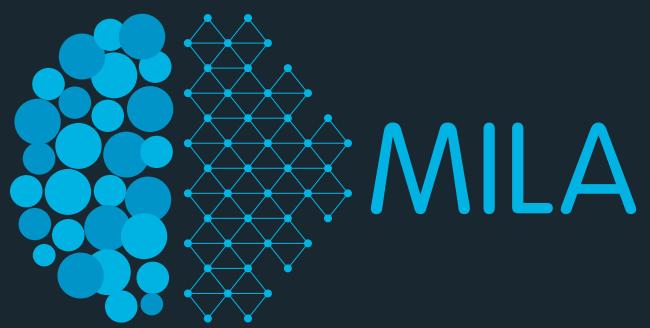
$$P(z) = \frac{1}{K} \sum_{i=1}^n \mathbb{1}_{\left( \frac{i-1}{n} \leq z \leq \frac{i}{n} \right)}^{a_i}$$

$$K = \sum_{i=1}^n K_i, \quad \text{where } K_0 := 0, K_i := \frac{a_i}{n} \text{ for } i = 1, \dots, n.$$



# Better Inference

# Suboptimality in Variational Inference

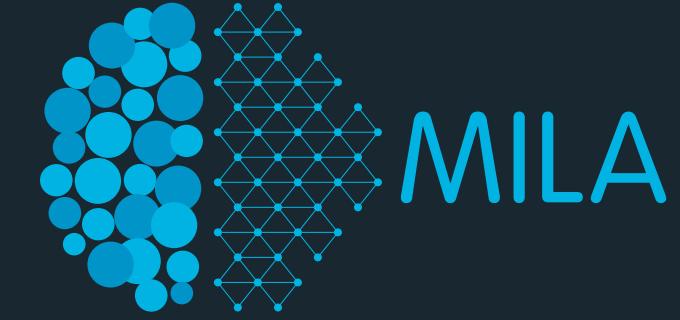


$$\log p_\theta(x) - \mathcal{L}(\theta, \phi; x) =$$

$$\underbrace{D_{\text{KL}}(q^* \| p)}_{\text{Gap 1}} + \underbrace{[D_{\text{KL}}(q_\theta^* \| p) - D_{\text{KL}}(q^* \| p)]}_{\text{Gap 2}} + \underbrace{[D_{\text{KL}}(q_\theta \| p) - D_{\text{KL}}(q_\theta^* \| p)]}_{\text{Gap 3}}$$

Dataset	MNIST				Fashion MNIST			
Variational Family	$q_{FFG}$	$q_{FFG}$	$q_{Flow}$	$q_{Flow}$	$q_{FFG}$	$q_{FFG}$	$q_{Flow}$	$q_{Flow}$
Encoder Capacity	Regular	Large	Regular	Large	Regular	Large	Regular	Large
$\log \hat{p}(x)$	-89.85	-89.09	-88.82	-88.59	-97.78	-94.55	-97.35	-96.16
$\mathcal{L}_{\text{VAE}}[q_{Flow}^*]$	-90.83	-90.05	-90.40	-90.26	-98.03	-95.93	-97.74	-96.87
$\mathcal{L}_{\text{VAE}}[q_{FFG}^*]$	-91.19	-90.34	-102.88	-103.53	-99.03	-98.09	-130.90	-129.24
$\mathcal{L}_{\text{VAE}}[q]$	-92.76	-91.12	-91.42	-91.25	-103.20	-101.28	-102.19	-100.60
Approximation	1.34	1.25	1.58	1.67	1.25	3.54	0.39	0.71
Amortization	1.57	0.78	1.02	0.99	4.17	3.19	4.45	3.73
Inference Gap	2.91	2.03	2.60	2.66	5.42	6.73	4.84	4.44

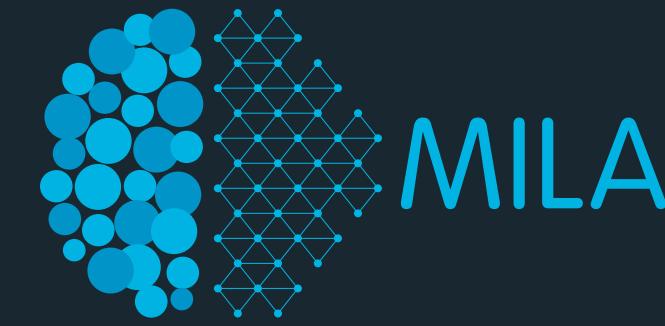
# Reducing Variational Gap



Methods that aim at reducing the variational gap (nonexhaustive)

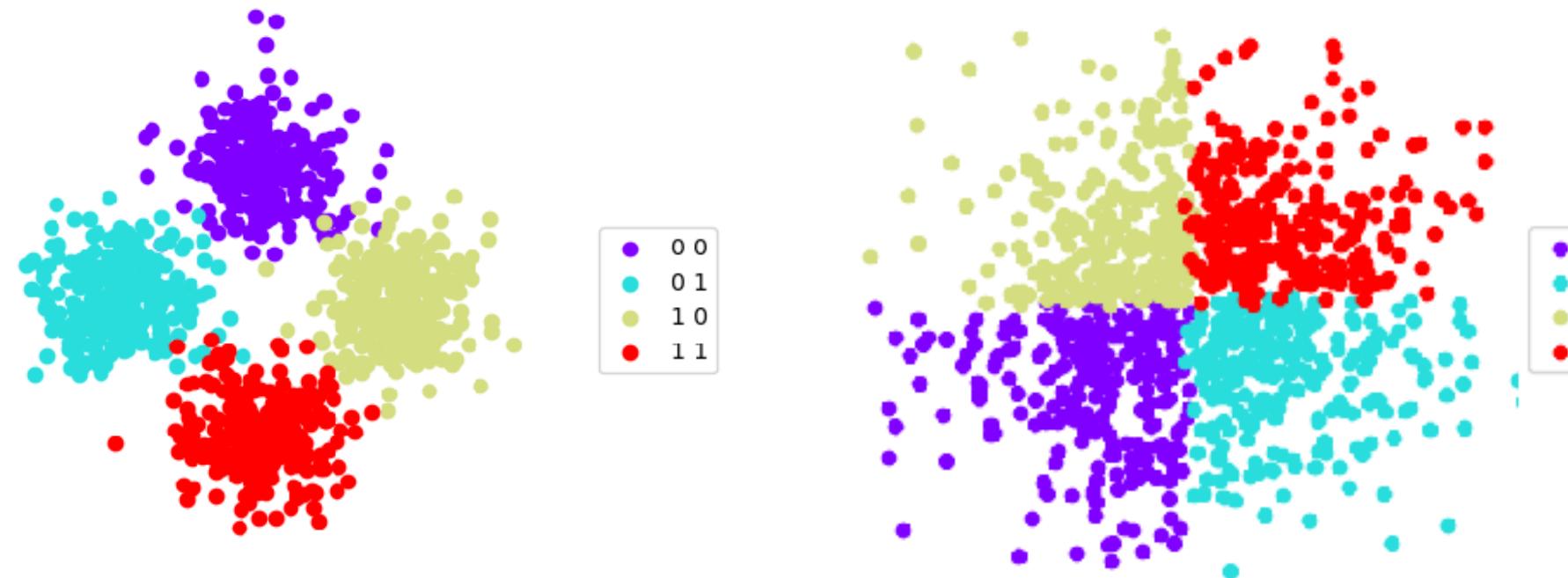
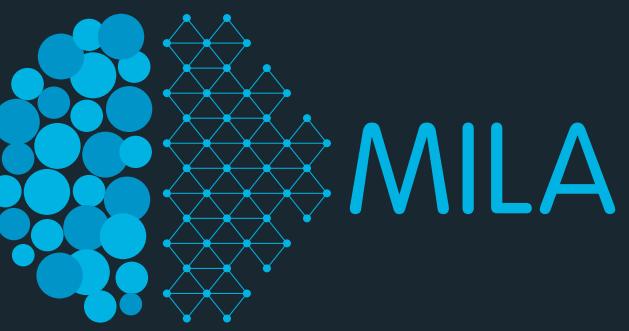
	Gap 1	Gap 2	Gap 3
Better optimization			✗
Better encoder [2]		✗	
Meta learning [10, 12, 8]		(✗)	(✗)
Normalizing flows [16, 9, 6]	✗		
Hierarchical VI [15, 11]	✗		
Implicit VI [13, 7]	✗		
Variational boosting [14]	✗		
MCMC as part of $q_\phi$ [17]	✗	✗	✗
MCMC on top of $q_\phi$ [3, 5]	(✗)	(✗)	(✗)
Gradient flow [4]	✗	✗	✗
Importance sampling [1]	(✗)	(✗)	(✗)

# Reducing Variational Gap Ref



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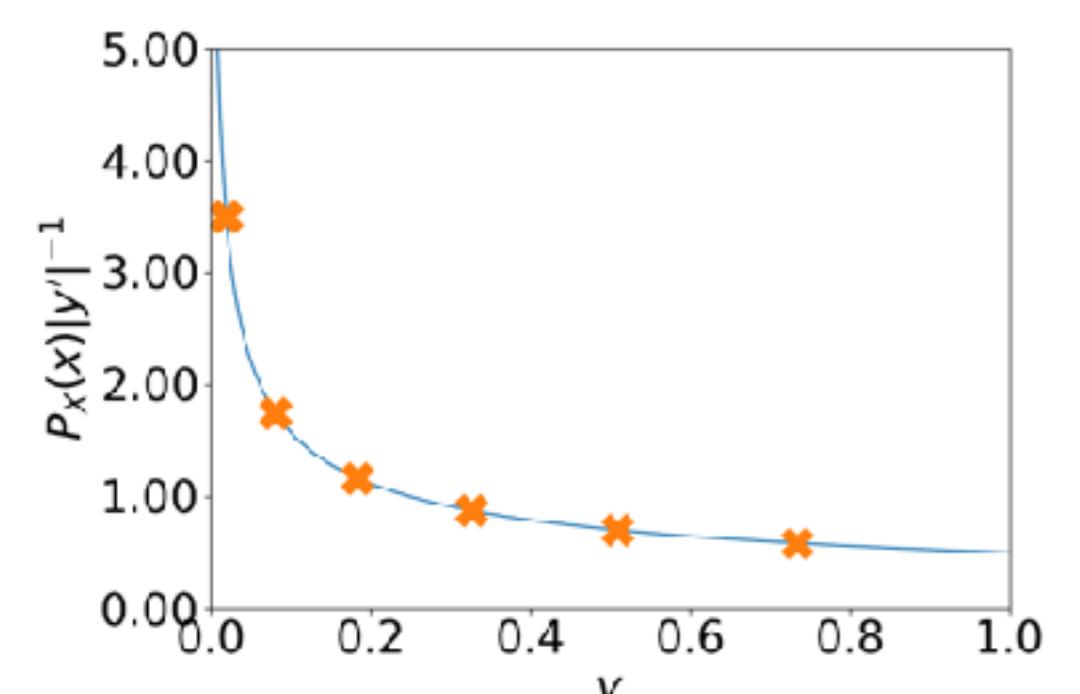
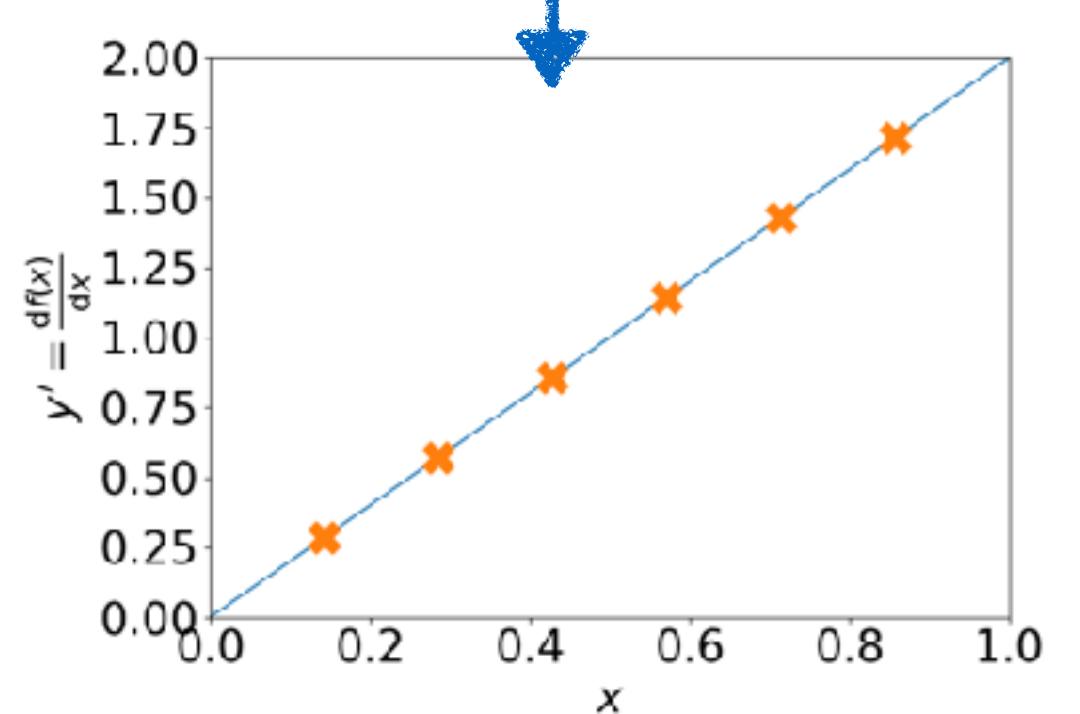
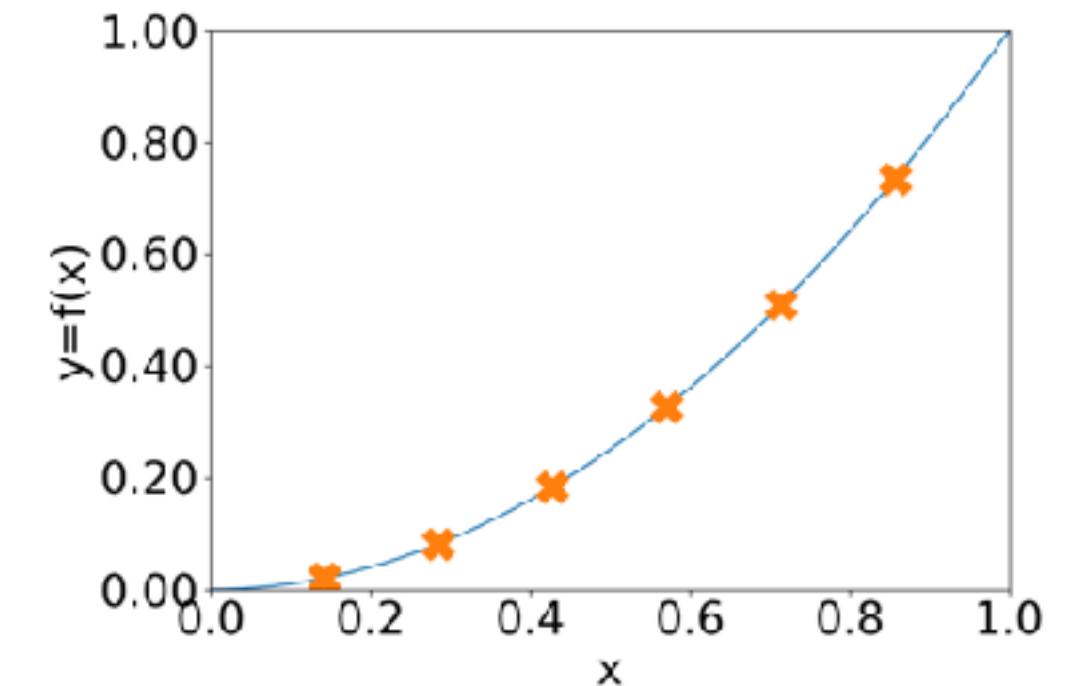
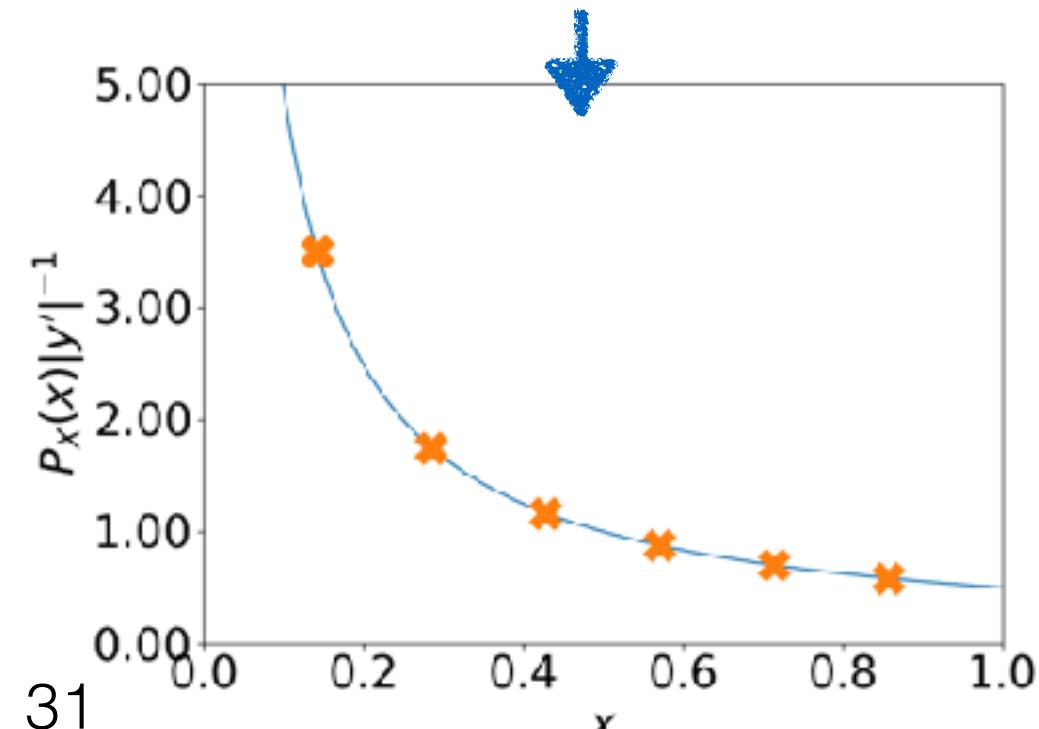
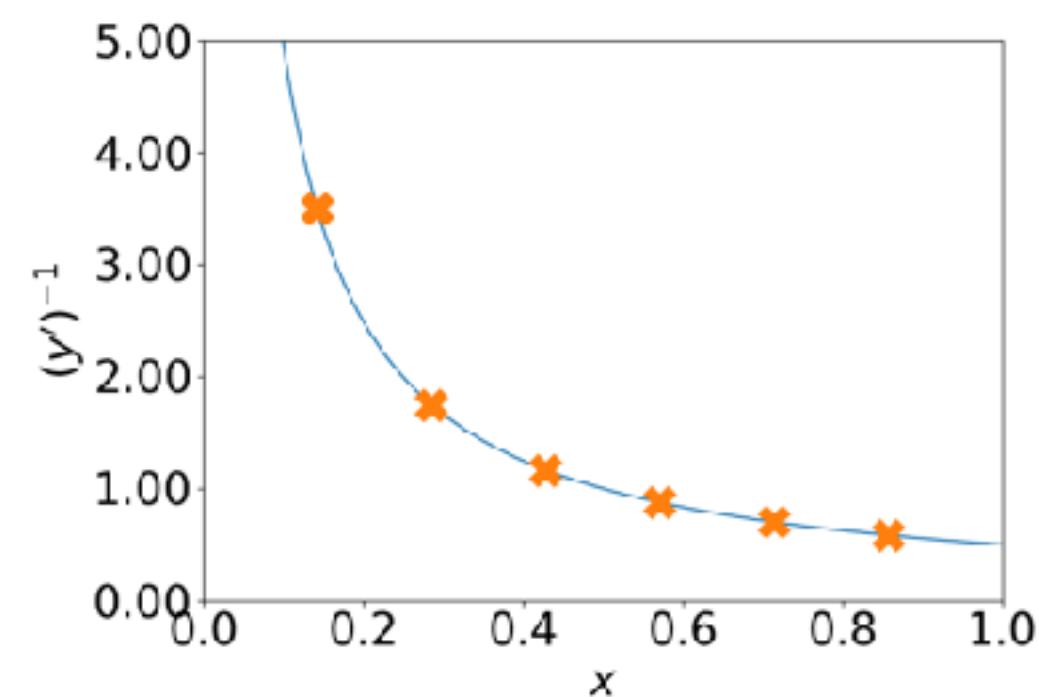
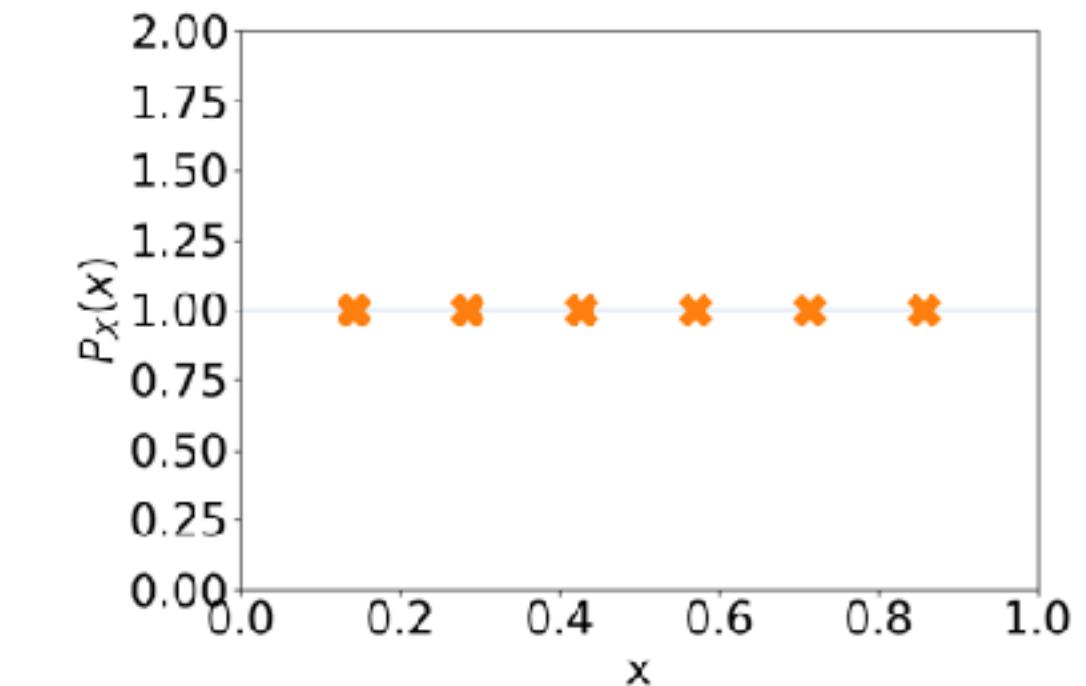
# Transformation Methods: Normalizing Flows



- Change of variable distribution

$$x \sim P_X(x); \quad y = f(x)$$

$$P_Y(y) = P_X(x) \left| \frac{df(x)}{dx} \right|^{-1}$$



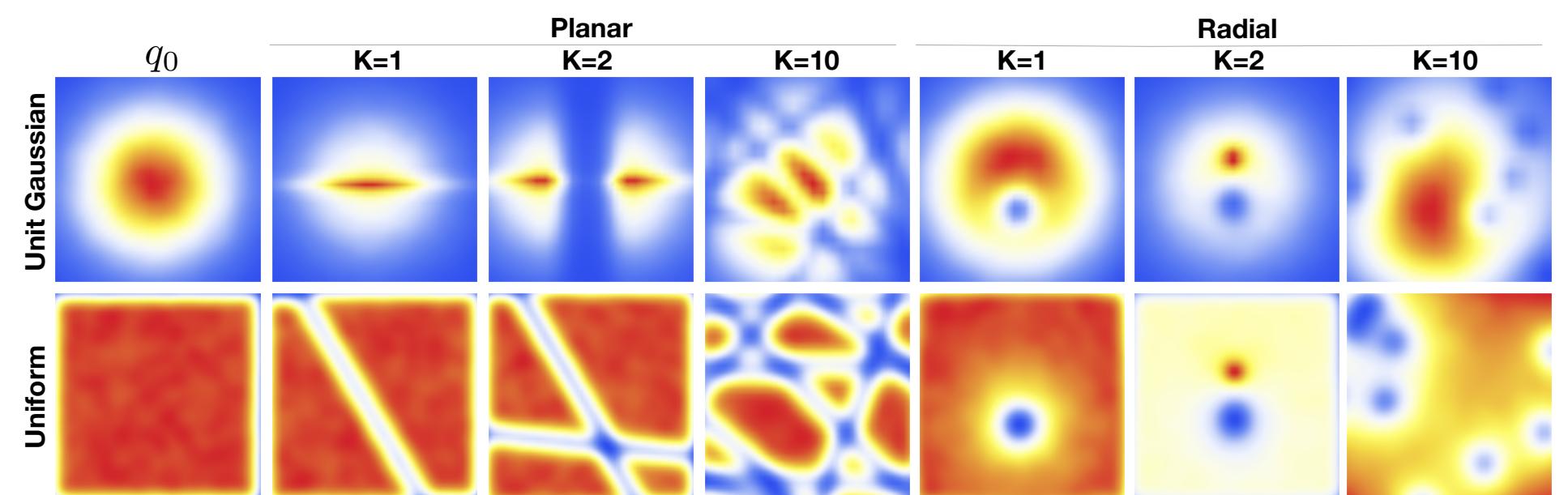
# Variational Inference with Normalizing Flows



- The density  $q_K(z)$  obtained by successively transforming a random variable  $z_0$  with distribution  $q_0$  through a chain of  $K$  transformations  $f_k$  is

$$z_K = f_K \circ \dots \circ f_2 \circ f_1(z_0)$$

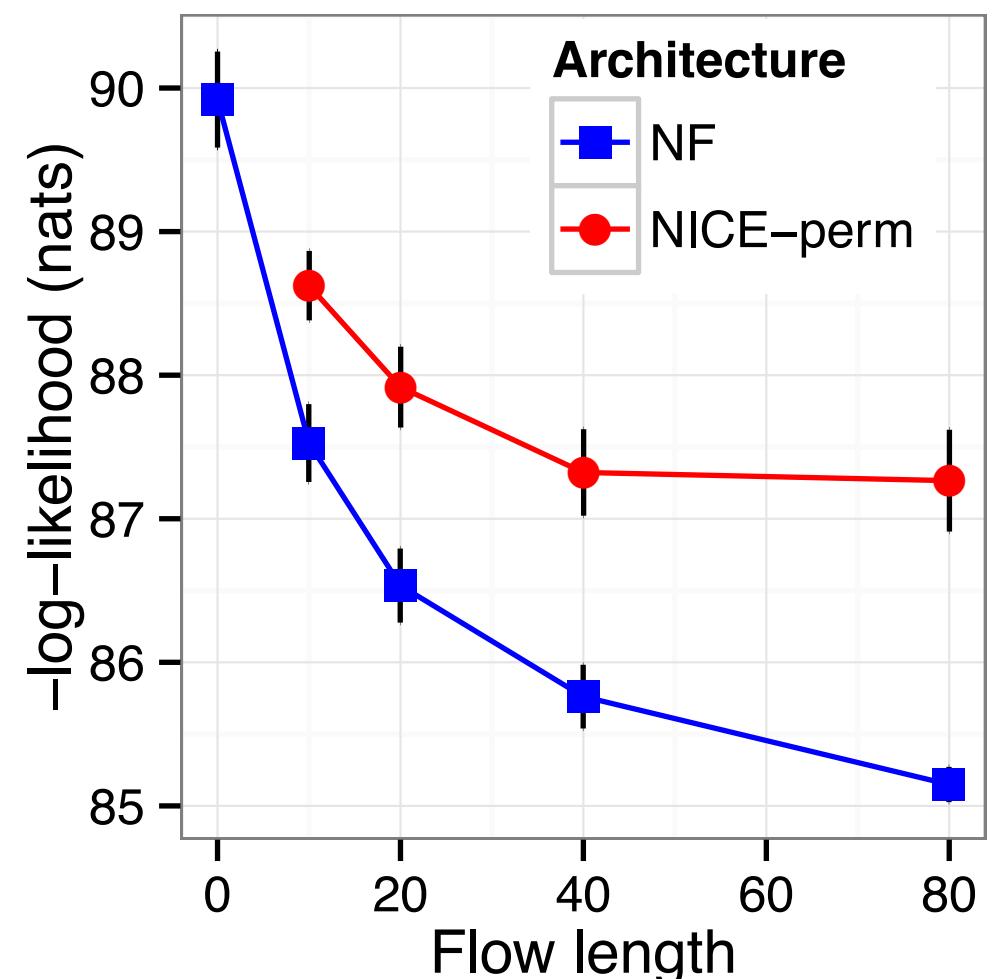
$$q_K(z_K) = \log q_0(z_0) - \sum_{k=1}^K \log \left| \det \frac{\partial f_k}{\partial z_{k-1}} \right|$$



- Law of unconscious statistician (LOTUS)

$$\mathbb{E}_{z_K} [h(z_K)] = \mathbb{E}_{z_0} [h(f_K \circ \dots \circ f_2 \circ f_1(z_0))]$$

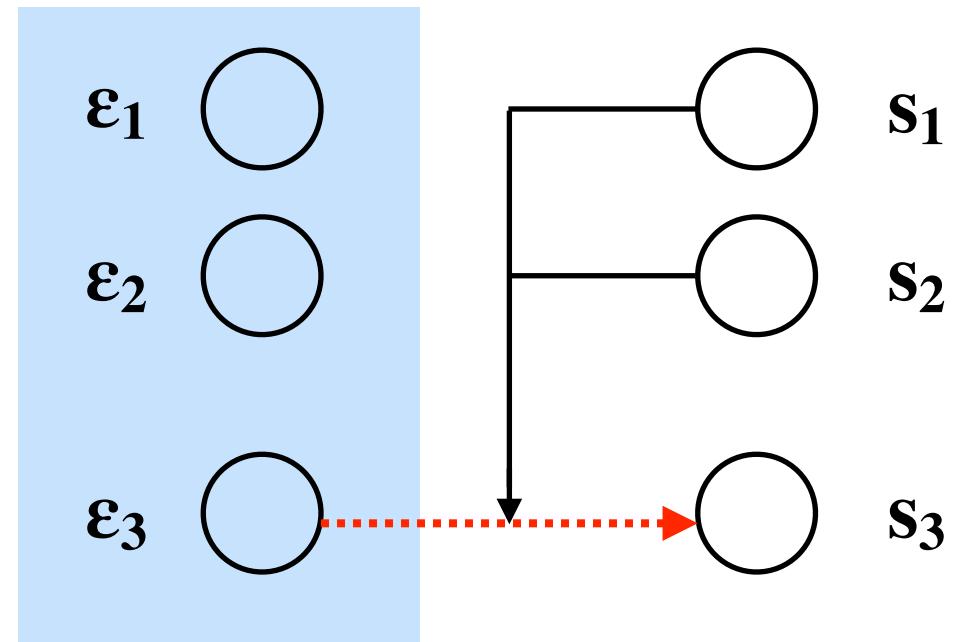
*How to rewrite the ELBO objective?*



# Inverse Autoregressive Flows

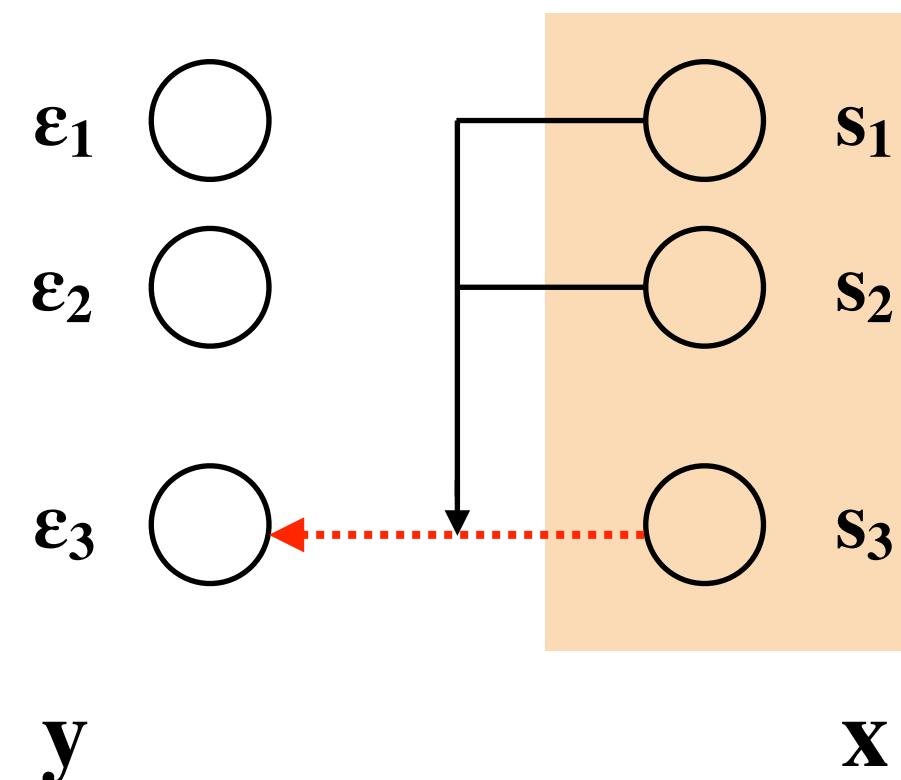


Unstructured noise Structured noise



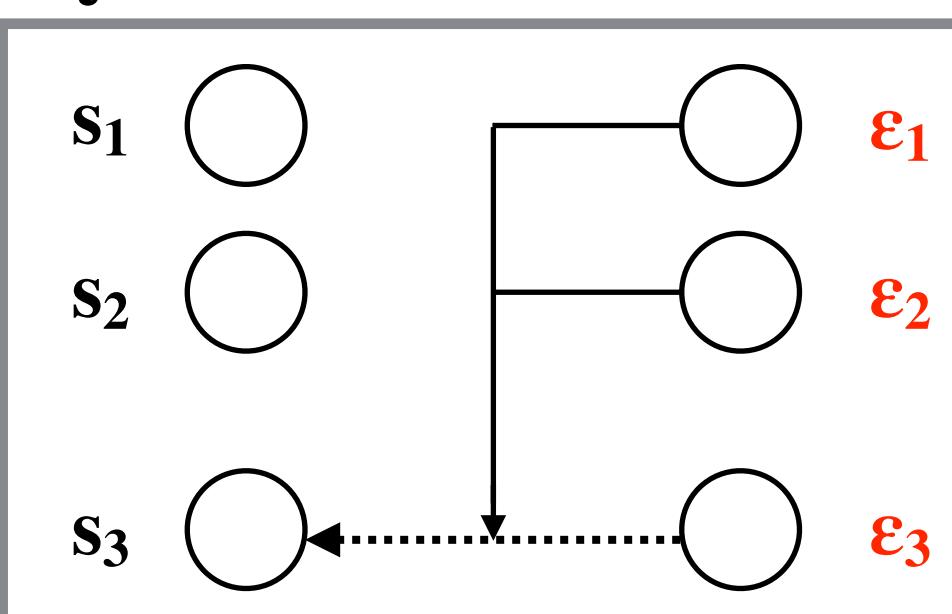
$$y_1 = \mu_1(\emptyset) + \sigma_1(\emptyset) \cdot \epsilon_1$$

$$y_j = \mu_j(y_{1:j-1}) + \sigma_j(y_{1:j-1}) \cdot \epsilon_j$$



$$\epsilon_1 = \frac{y_1 - \mu_1(\emptyset)}{\sigma_1(\emptyset)}$$

$$\epsilon_j = \frac{y_j - \mu_j(y_{1:j-1})}{\sigma_j(y_{1:j-1})}$$



- Change of variable distribution

$$x \sim P_X(x); \quad y = f(x)$$

$$P_Y(y) = P_X(x) \left| \frac{df(x)}{dx} \right|^{-1}$$

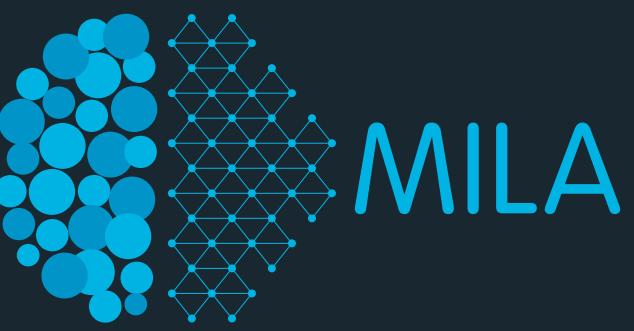
## Autoregressive model

$$p(y_{1:P}) = p(y_1) \prod_{j=2}^P p(y_j|y_{1:j-1})$$

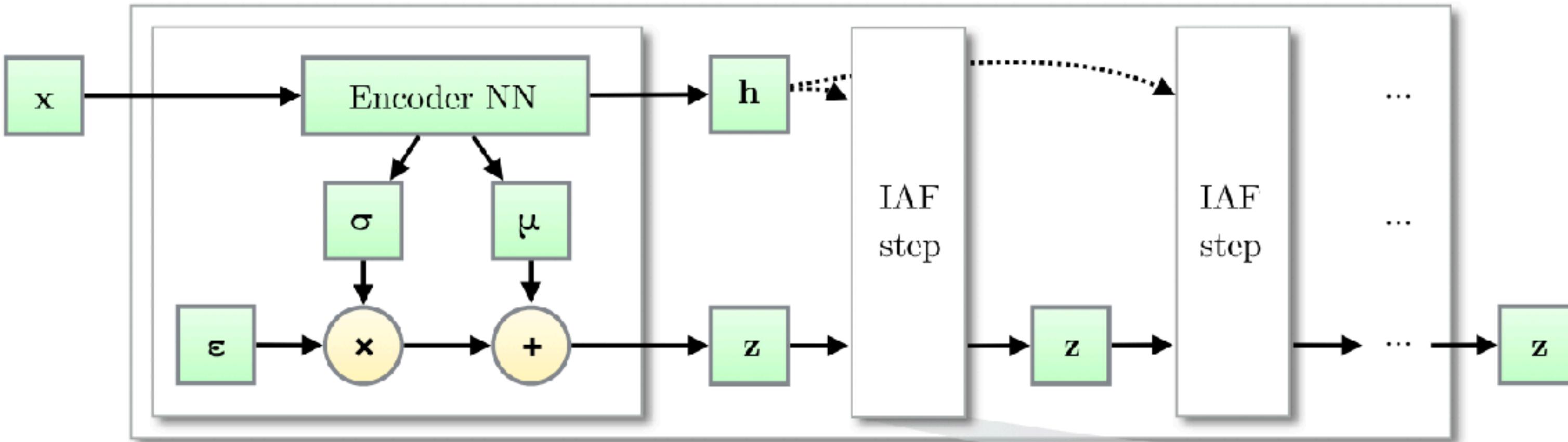
$$= \mathcal{N}(y_1; \mu_1, \sigma_1^2) \prod_{j=2}^P \mathcal{N}(y_j | \mu_j(y_{1:j-1}), \sigma_j^2(y_{1:j-1}))$$

- *Scales well to high-dimensional space in terms of complexity (no rank-one restriction)*
- *Linear complexity in computing log determinant of Jacobian (upper triangular Jacobian)*
- *No dependency in sampling (non-sequential)*
- *More expressive than pure autoregressive model (composable)*

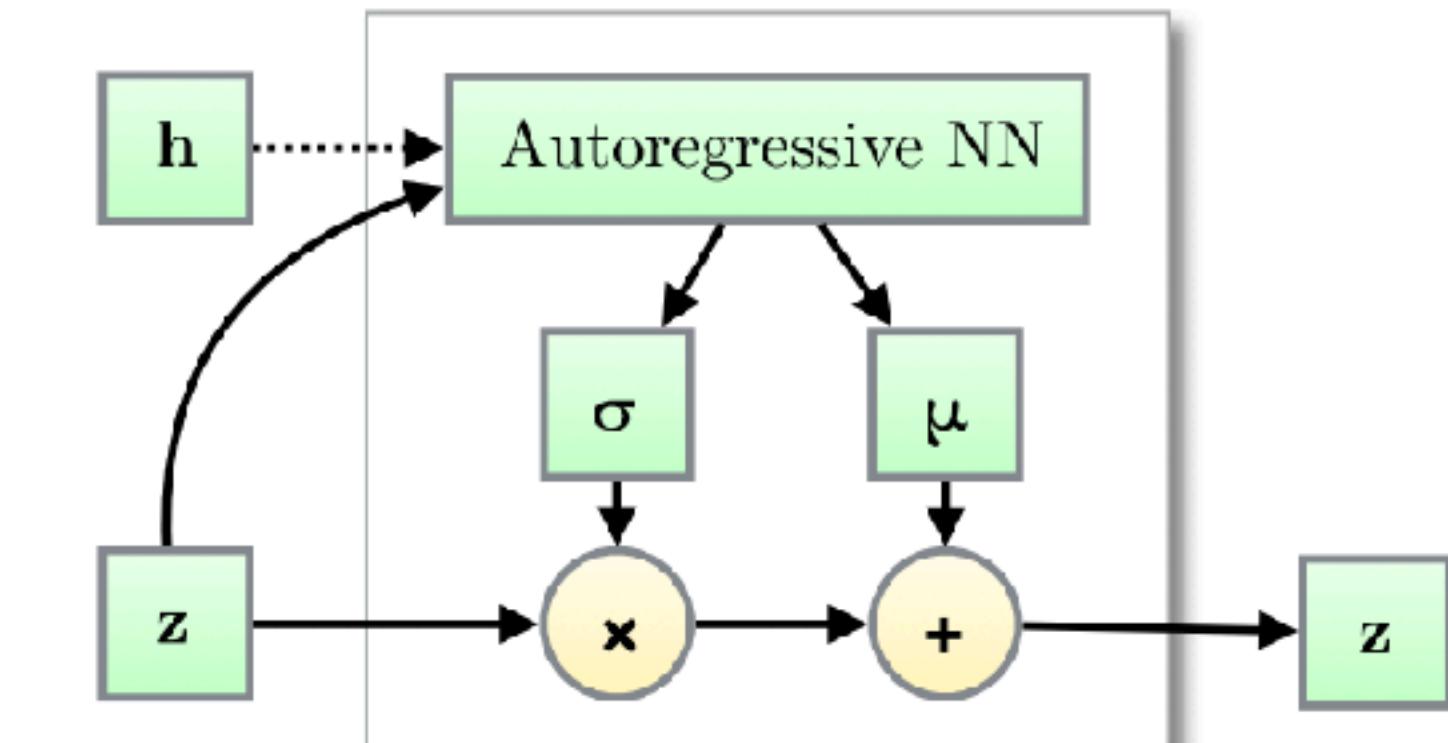
# Improving Variational Inference with IAF



Approximate Posterior with Inverse Autoregressive Flow (IAF)



IAF Step



Non-affine

$$\epsilon \sim \mathcal{N}(0, \mathbf{I})$$

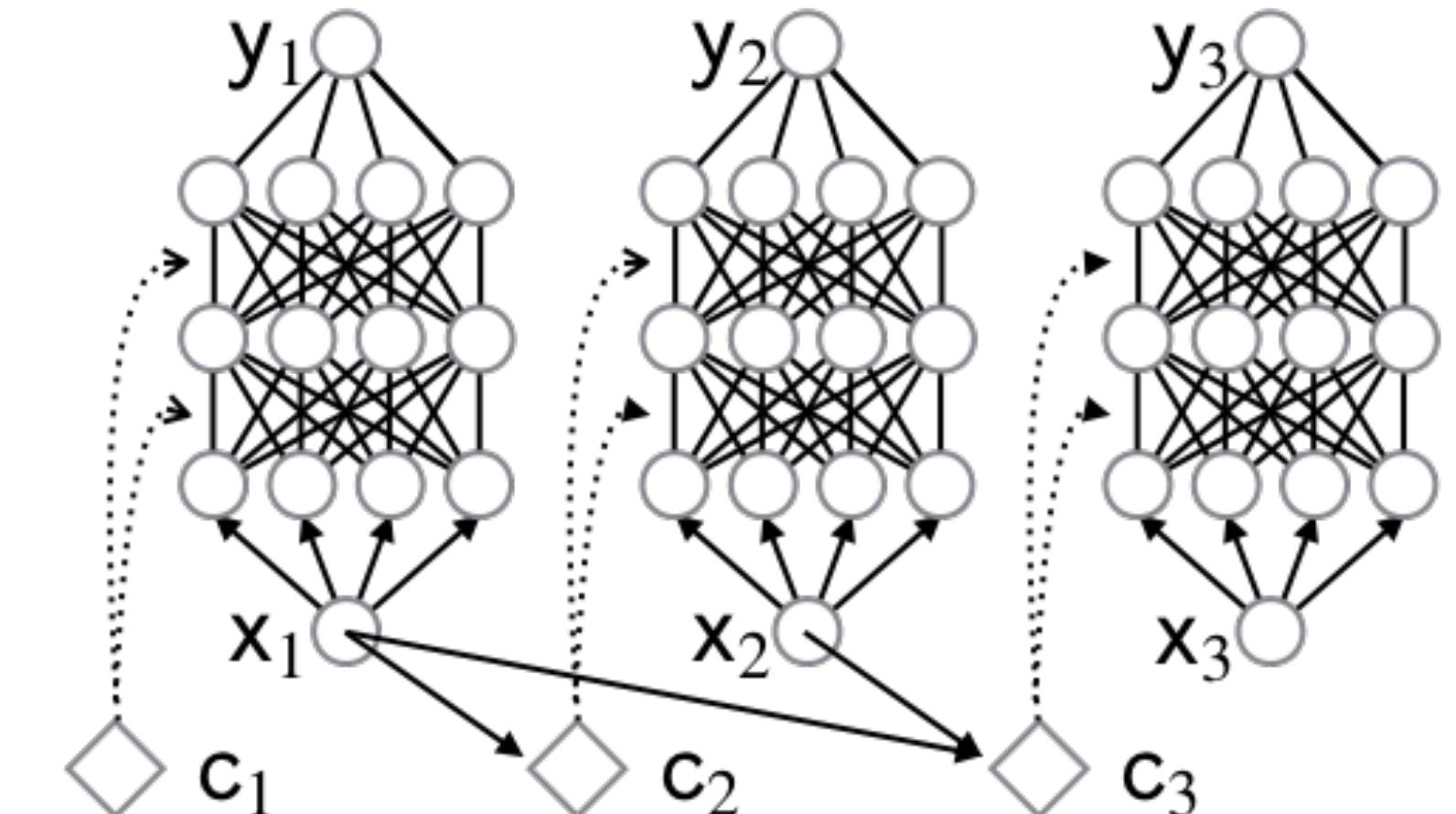
$$z_0 = \mu_0(x) + \sigma_0(x) \odot \epsilon$$

$$z_k = \mu_k(z_{k-1}) + \sigma_k(z_{k-1}) \odot z_{k-1}$$

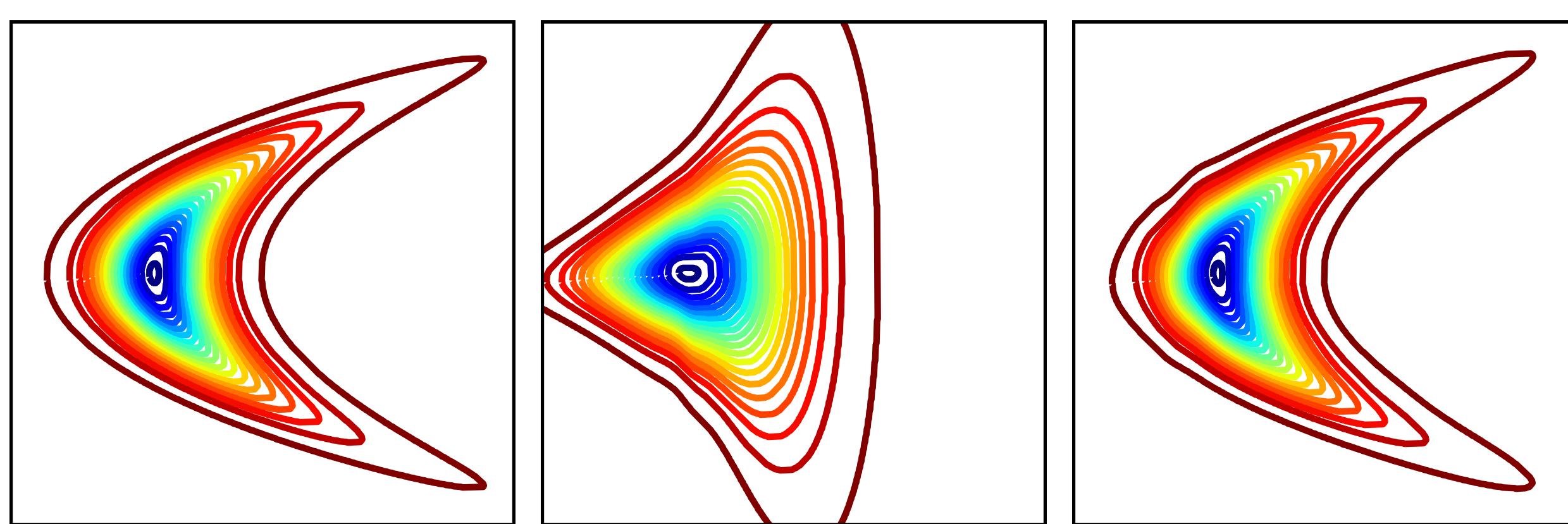
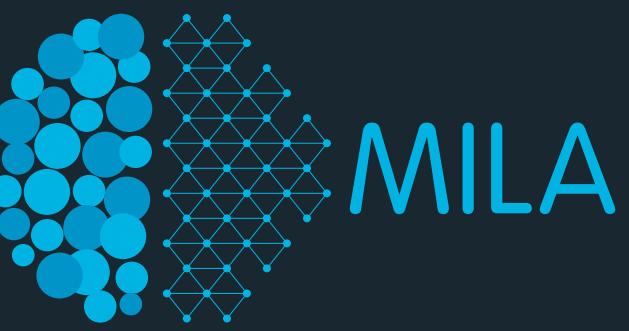
Method	bits/dim $\leq$
Multivariate Gaussian (van den Oord et al., 2016b)	4.70
NICE (Dinh et al., 2014)	4.48
Deep GMMs (van den Oord and Schrauwen, 2014)	4.00
Real NVP (Dinh et al., 2016)	3.49
PixelRNN (van den Oord et al., 2016b)	<b>3.00</b>
Gated PixelCNN (van den Oord et al., 2016c)	<b>3.03</b>

Results with variationally trained latent-variable models:

Deep Diffusion (Sohl-Dickstein et al., 2015)	5.40
Convolutional DRAW (Gregor et al., 2016)	3.58
ResNet VAE with IAF (Ours)	<b>3.11</b>



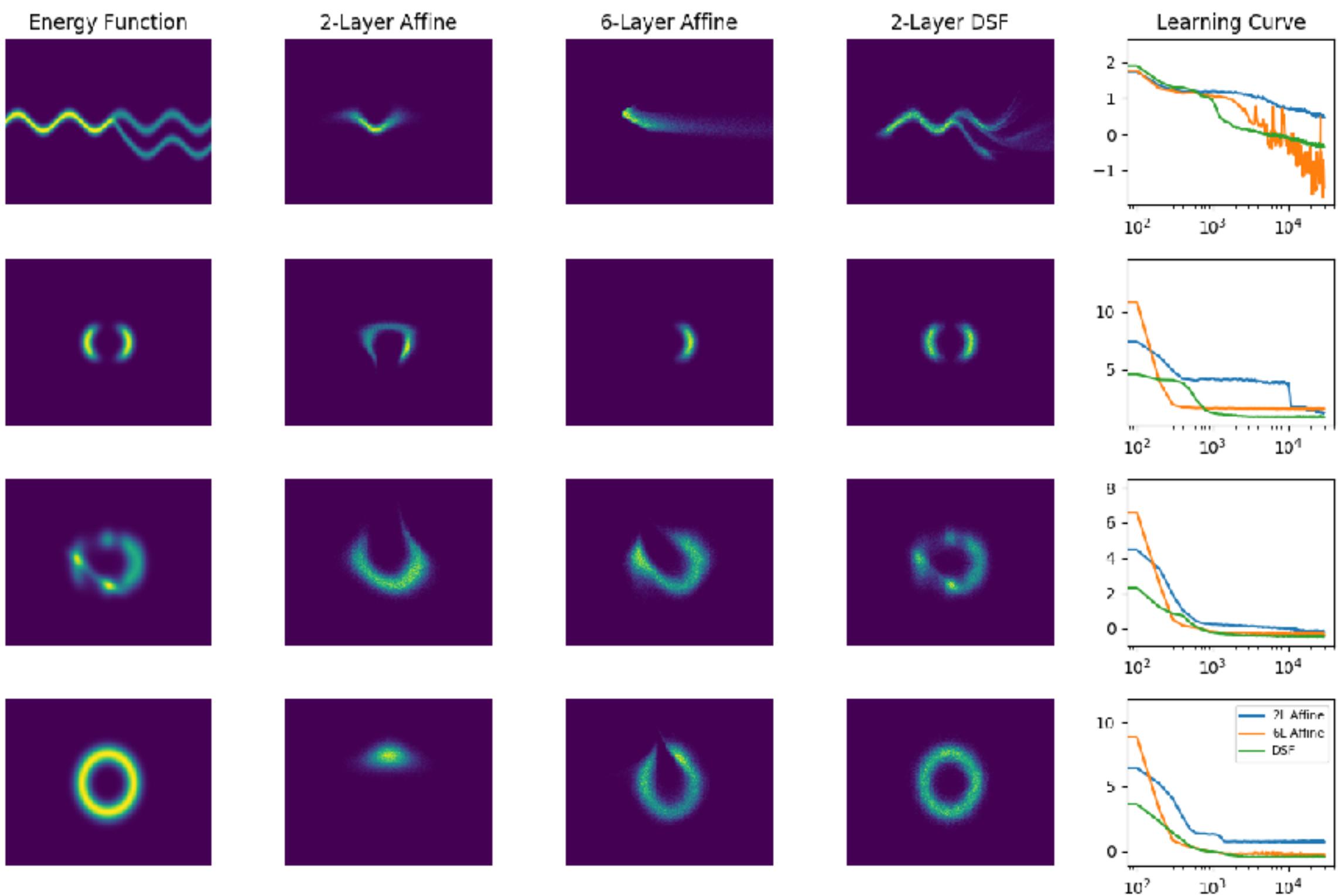
# Expressiveness of Autoregressive Flows



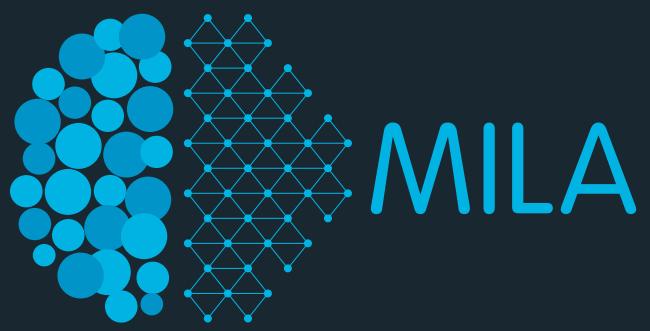
Target

MADE

5 MADEs



# Importance Weighted Autoencoders



$$\mathcal{L}_k(x) = \mathbb{E}_{z_{1:k} \sim q(z|x)} \log \frac{1}{k} \sum_{i=1}^k \underbrace{\frac{p(x, z_i)}{q(z_i|x)}}_{w_i}$$

$$\nabla \mathcal{L}_k(x) = \mathbb{E}_{\epsilon_{1:k}} \left[ \sum_{i=1}^k \tilde{w}_i \nabla \log w_i \right]$$

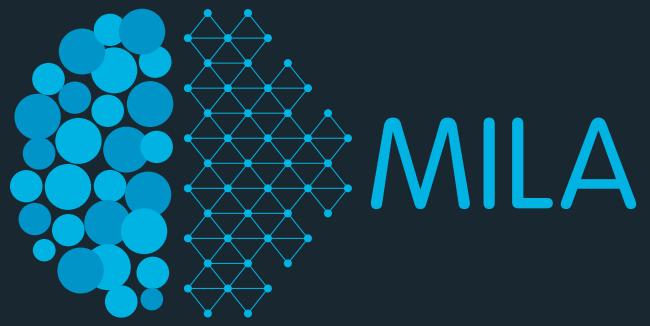
# stoch. layers	k	MNIST		IWAE	
		VAE NLL	active units	IWAE NLL	active units
1	1	86.76	19	86.76	19
	5	86.47	20	85.54	22
	50	86.35	20	84.78	25
2	1	85.33	16+5	85.33	16+5
	5	85.01	17+5	83.89	21+5
	50	84.78	17+5	82.90	26+7

**Theorem 1.** For all  $k$ , the lower bounds satisfy

$$\log p(\mathbf{x}) \geq \mathcal{L}_{k+1} \geq \mathcal{L}_k.$$

Moreover, if  $p(\mathbf{h}, \mathbf{x})/q(\mathbf{h}|\mathbf{x})$  is bounded, then  $\mathcal{L}_k$  approaches  $\log p(\mathbf{x})$  as  $k$  goes to infinity.

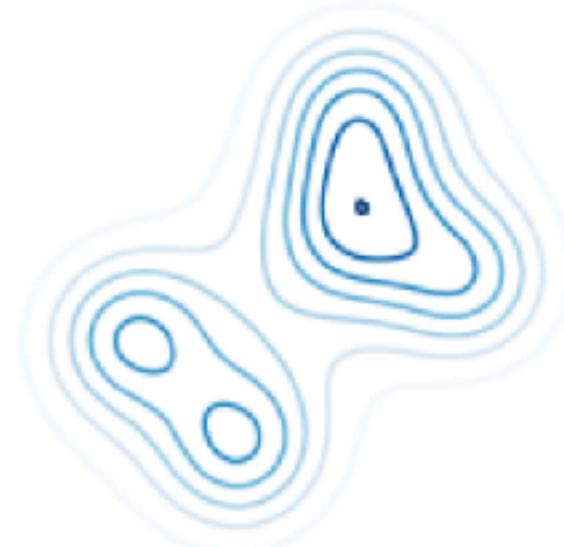
# Iterative Refinement with Importance Sampling



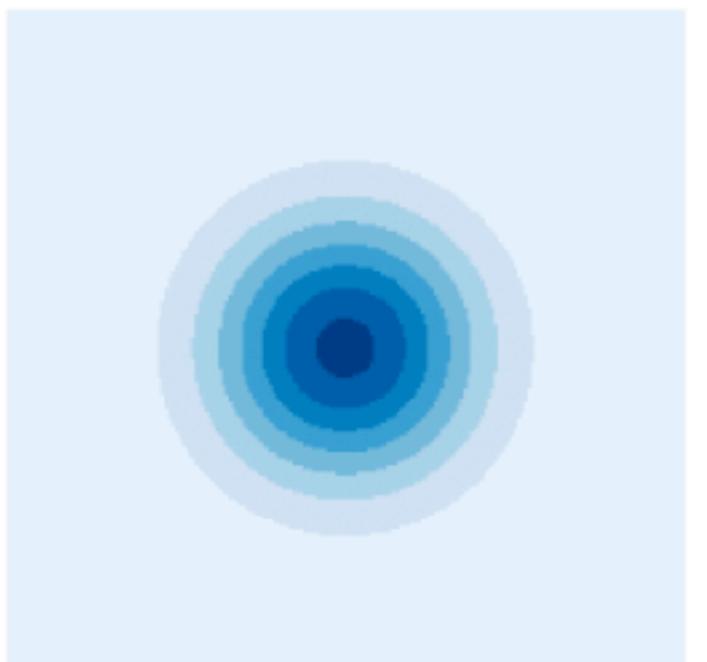
$$q_{IW}(z|x) = E_{z_2 \dots z_k \sim q(\cdot|x)} \left[ \frac{p(x, z)}{\frac{1}{k} \left( \frac{p(x, z)}{q(z|x)} + \sum_{j=2}^k \frac{p(x, z_j)}{q(z_j|x)} \right)} \right]$$

$$\mathcal{L}_{VAE}[q_{IW}] = \dots = E_{z_1 \dots z_k \sim q(z|x)} \left[ \log \left( \frac{1}{k} \sum_{j=1}^k \frac{p(x, z_j)}{q(z_j|x)} \right) \right] = \mathcal{L}_{IWAE}[q]$$

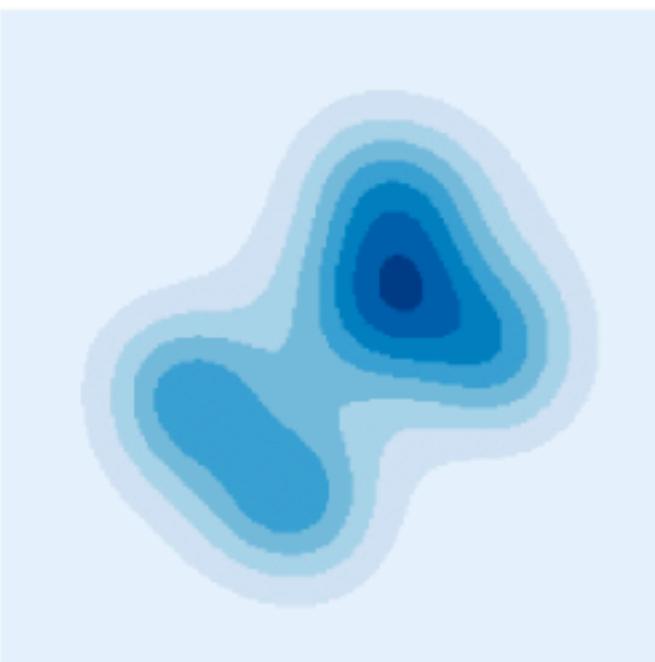
True posterior



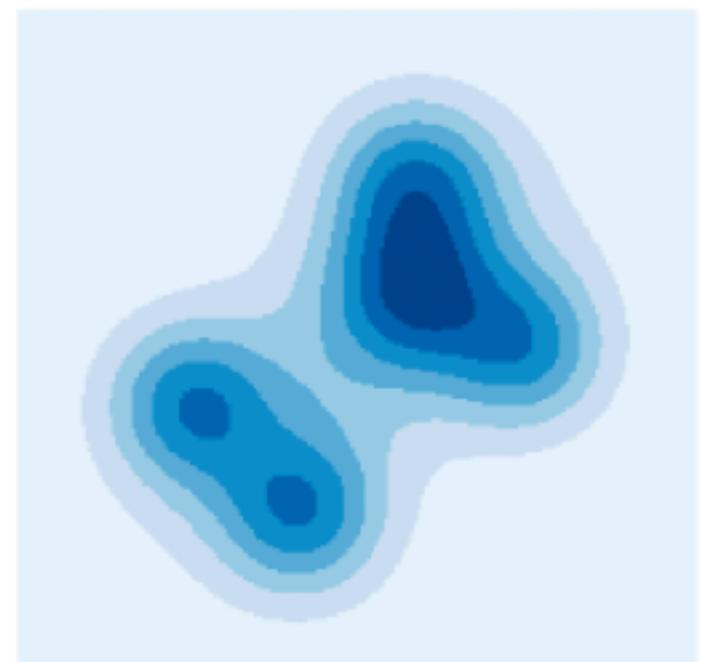
$q_{IW}$  with  $k = 1$



$q_{IW}$  with  $k = 10$



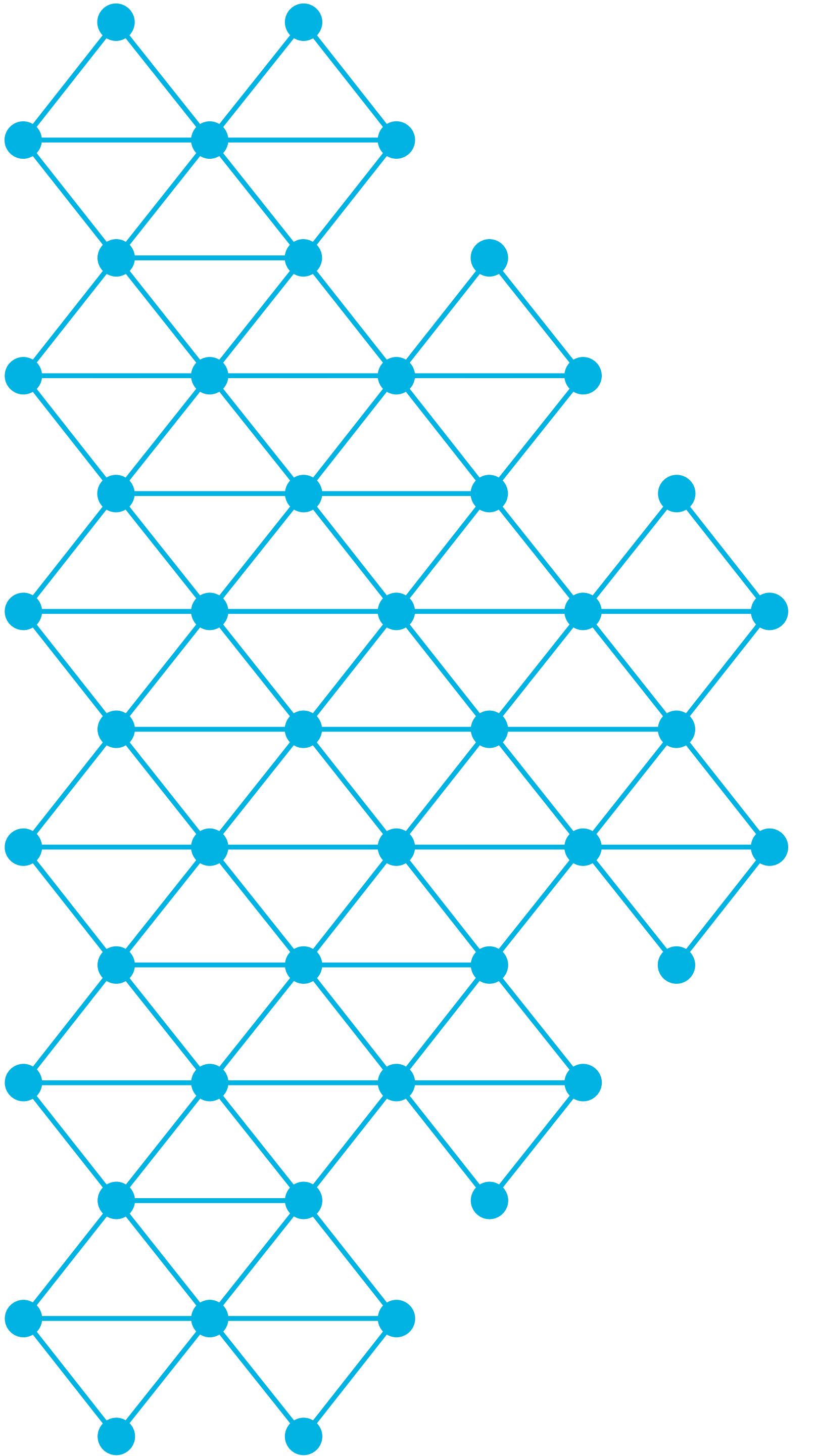
$q_{IW}$  with  $k = 100$



# Summary

We've talked about ...

- Using latent variable models (deep latent gaussian models) as generative models;
  - Variational Bayes, ELBO
- Using an encoder to amortize inference
- Using reparameterization trick to reduce variance in gradient estimate; to make stochastic backward propagation possible
- How to improve model assumption using non fully factorized gaussian distribution as prior or likelihood
- How to improve inference using better inference network (e.g. larger capacity or meta learning)
- How to improve inference using transformation methods, or sampling methods



# Reference

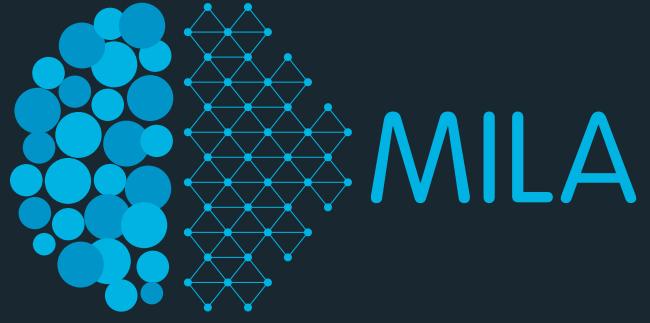
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