Institut
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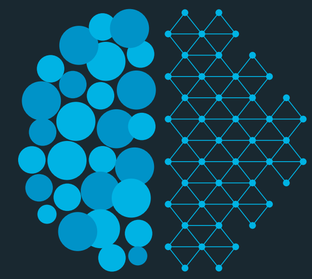


Variational Autoencoders

Chin-Wei Huang

Autoencoders as Generative Models

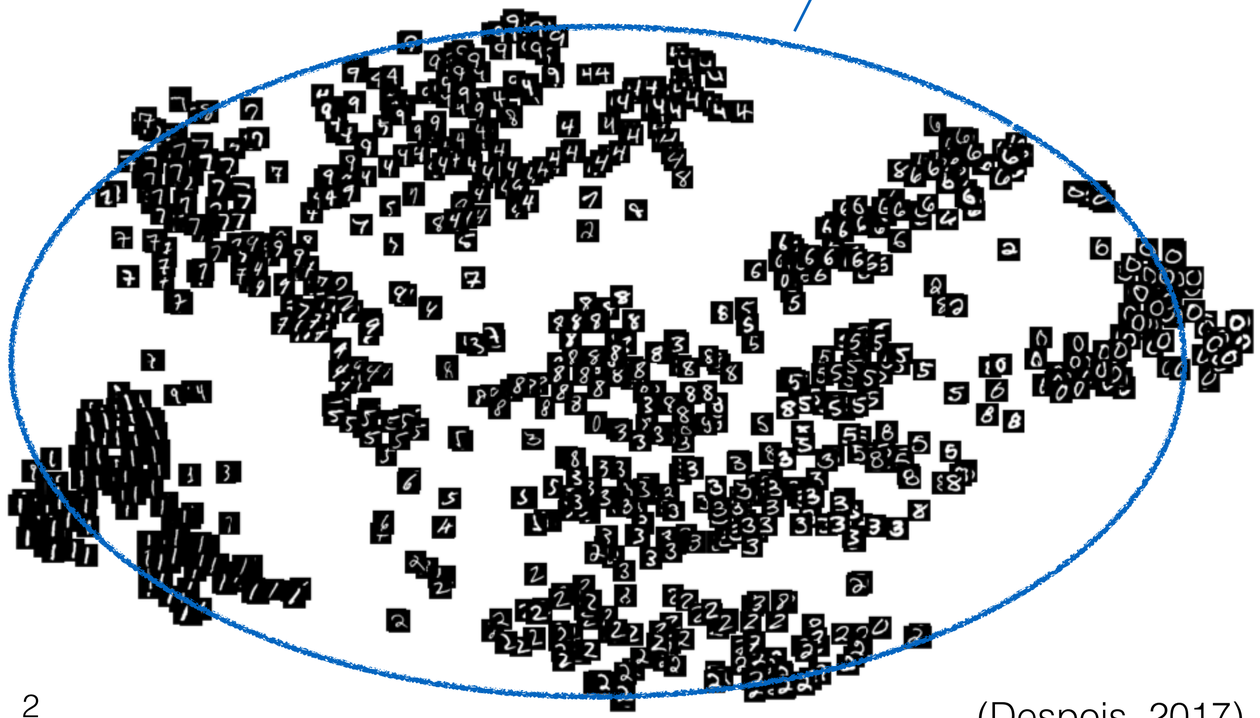
- Regularized autoencoder's objective:

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

parameters

code

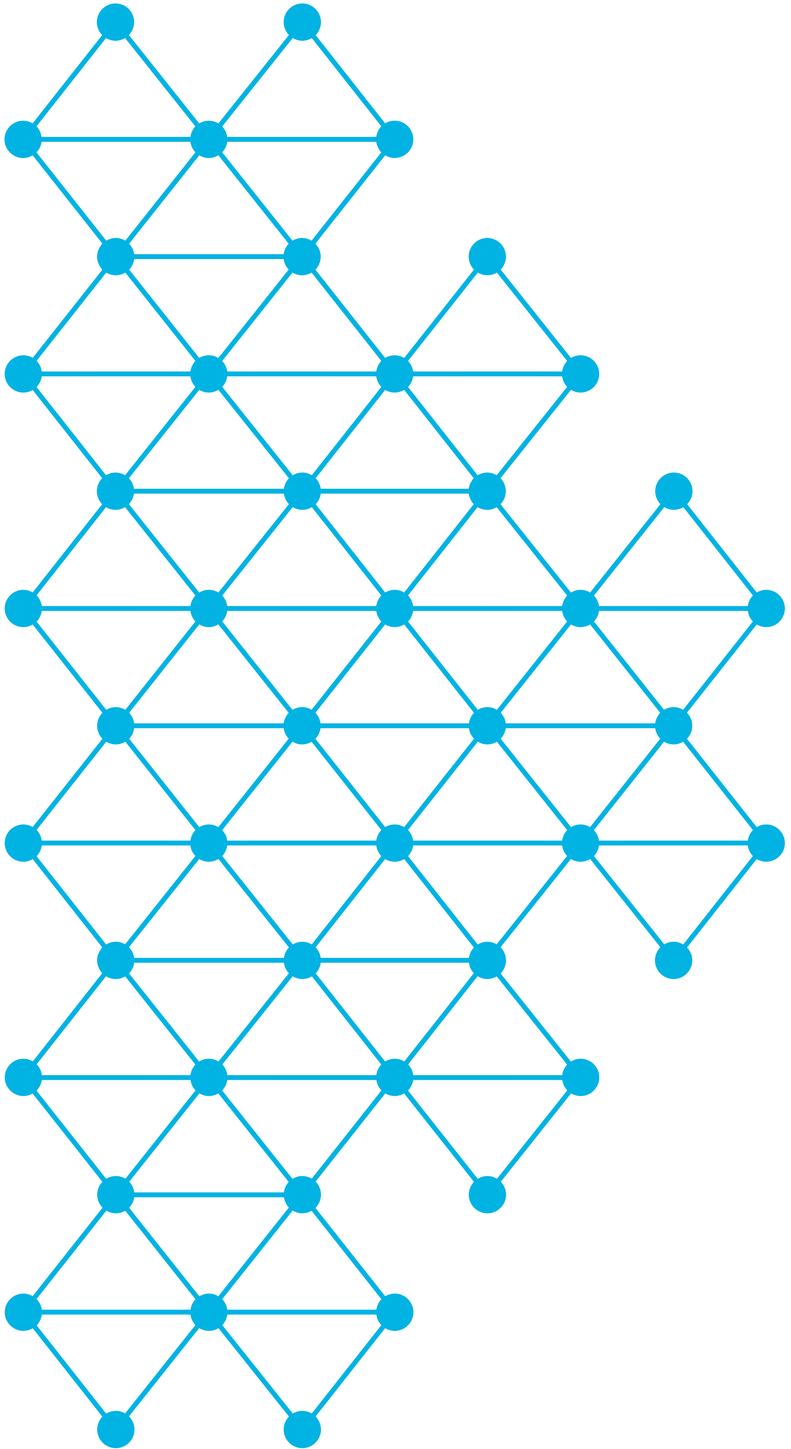
$$z \sim p(z); \quad x = h_\theta(z)$$



(Despois, 2017)

Overview

- **Background**
  - Recap: MLE, maximum marginal likelihood, EM
- **Variational Inference and VAE**
  - Approximate inference
  - 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)?

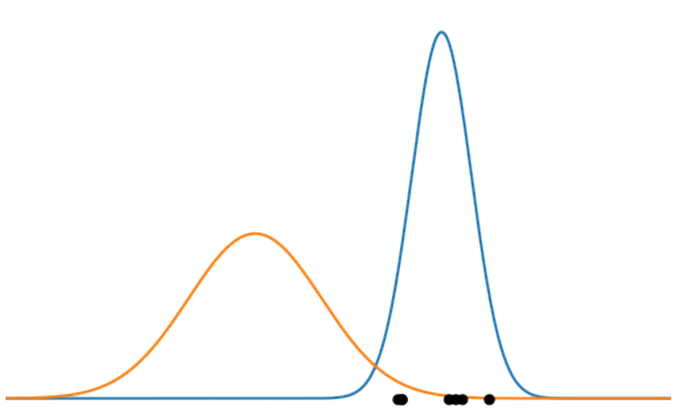


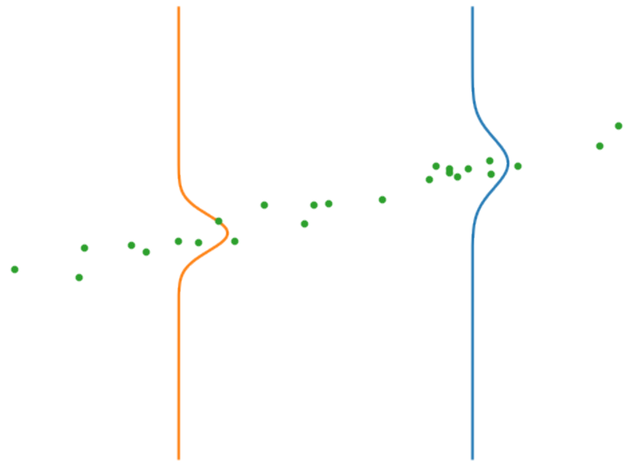
Background

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;

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

- 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):

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

$$\text{E step:} \quad q_{t+1} \leftarrow \operatorname*{argmax}_q \mathcal{L}(p_t, q) = p_t(z|x)$$

$$\text{M step:} \quad p_{t+1} \leftarrow \operatorname*{argmax}_p \mathcal{L}(p, q_{t+1})$$

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

Approximate Inference

The need of approximate inference

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

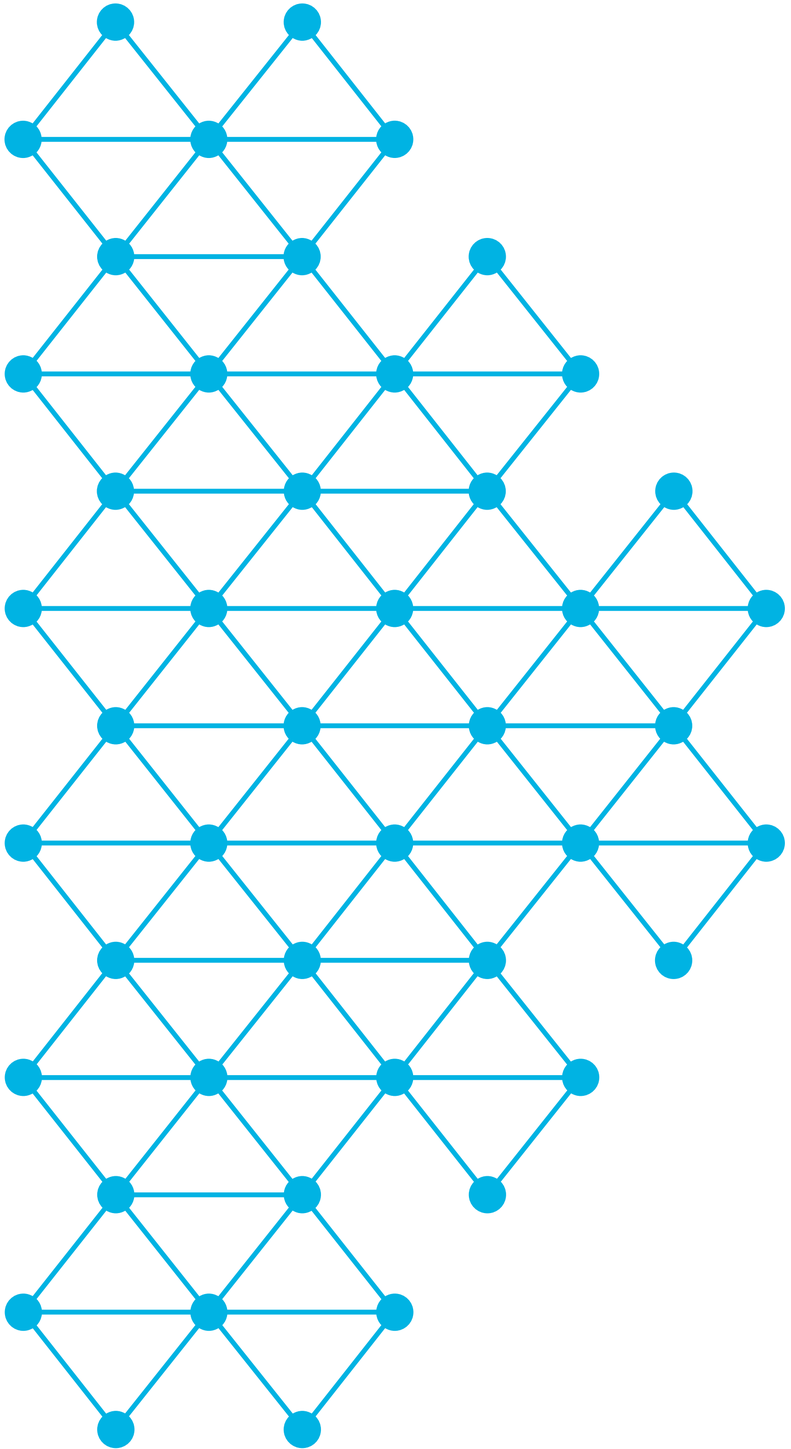
make a guess!

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. $p(z) = \mathcal{N}(z; 0, \mathrm{I})$
2. $x \sim p(x|z) = p(x; \mathrm{dec}(z))$; e.g. $p(x|z) = \mathrm{Bern}(x; \pi(z))$

$$\log p(x) = \log \int_z p(x|z)p(z)\mathrm{d}z$$

$$= \log \int_z p(x|z)\frac{p(z)}{q(z)}q(z)\mathrm{d}z$$

$$= \log \mathbb{E}_{z\sim q(z)}\left[p(x|z)\frac{p(z)}{q(z)}\right]$$

$$\geq \mathbb{E}_{z\sim q(z)}\left[\log p(x|z)\frac{p(z)}{q(z)}\right]$$

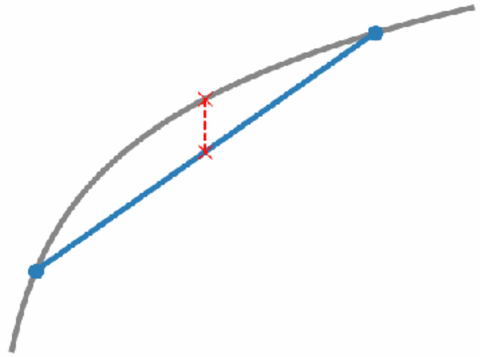
$$= \mathbb{E}_{z\sim q(z)}\left[\log p(x,z) - \log q(z)\right]$$

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

$$\frac{q(z)}{q(z)} = 1$$

log is concave;

Jensen's Inequality



Jordan et al., 1999
Wainwritght and Jordan, 2008
Blei et al., 2017

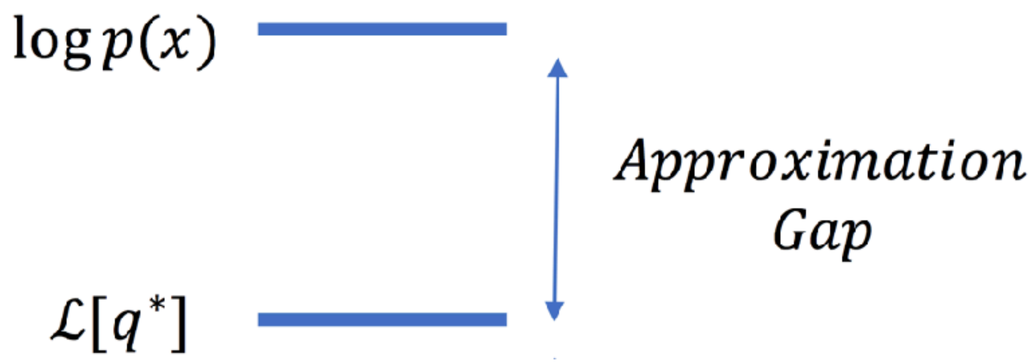
Variational Gap

$$\log p(x) - \overbrace{\mathbb{E}_{z\sim q(z)}\left[\log p(x,z) - \log q(z)\right]}^{\mathcal{L}(p,q)}$$

$$= \mathbb{E}_{z\sim q(z)}[\log q(z) - \log \frac{p(x,z)}{p(x)}]$$

$$= \mathbb{E}_{z\sim q(z)}[\log q(z) - \log p(z|x)]$$

$$= D_{\mathrm{KL}}\left(q(z)\|p(z|x)\right)$$



(Cremer et al. 2017)

Amortized Variational Inference

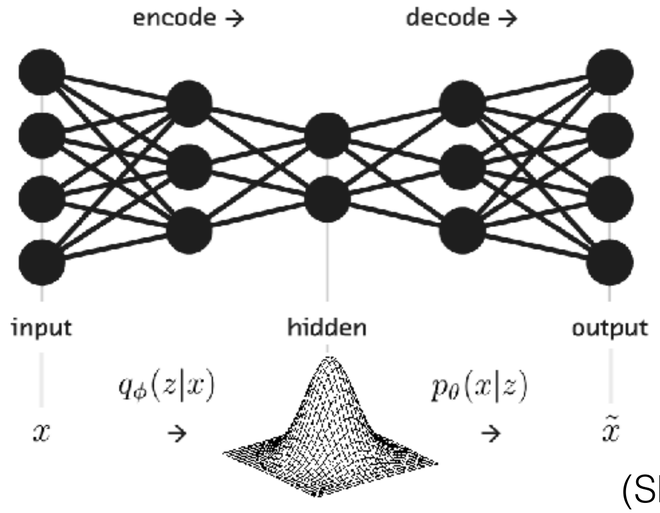
Traditional VI

- 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) $q_\phi(z|x_i)$

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



(Shiffman et al., 2016)

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)

$$\nabla \mathcal{L}_i = \mathbb{E}_z \left[(\log p(x_i, z) - \log q(z|x_i)) \nabla \log q(z|x_i) \right]$$

$$\approx \frac{1}{M} \sum_{m=1}^{M} (\log p(x_i, z_m) - \log q(z_m|x_i)) \nabla \log q(z_m|x_i) \qquad z_m \sim q(z|x_i)$$

unbiased, high variance

Remedies:
- More samples
- Rao-Blackwellization
- Control Variate
- Baseline …

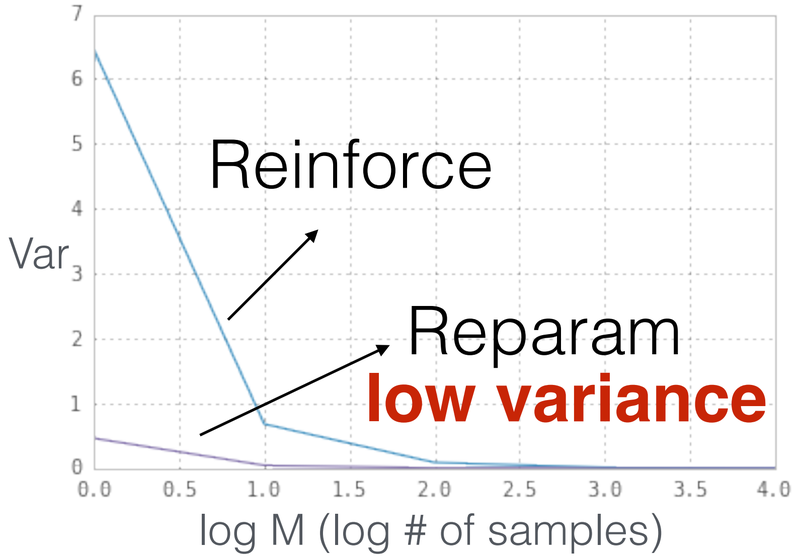
Other gradient estimator?

Black-Box Variational Inference (Ranganath et al., 2014)
NVIL (Mnih & Gregor, 2014)

Reparameterization Trick

- Decompose the sampling process into

$$z \sim q_\phi(z|x) \quad \Leftrightarrow \quad \epsilon \sim q(\epsilon);$$
$$z = g_\phi(\epsilon, x)$$
$$z \sim \mathcal{N}(z; \mu_\phi(x), \sigma^2_\phi(x)) \quad \Leftrightarrow \quad \epsilon \sim \mathcal{N}(\epsilon; 0, \mathrm{I});$$
$$z = \sigma(x) \odot \epsilon + \mu(x)$$



How to estimate the gradient then?

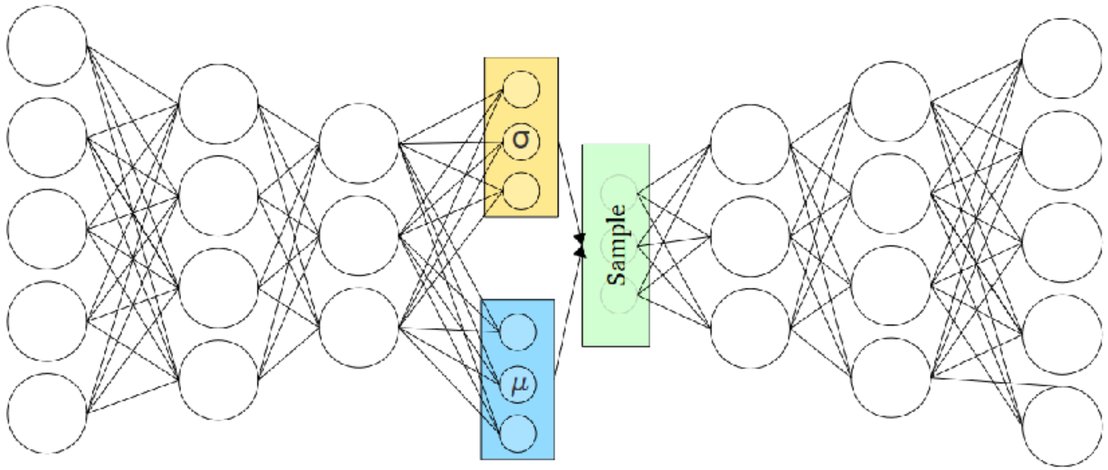
Doubly Stochastic Variational Bayes (Titsias & Lazaro-Gredilla, 2014)
Stochastic Gradient Variational Bayes, SGVB (Kingma & Welling, 2014)
Stochastic Backpropagation (Rezende et al, 2014)

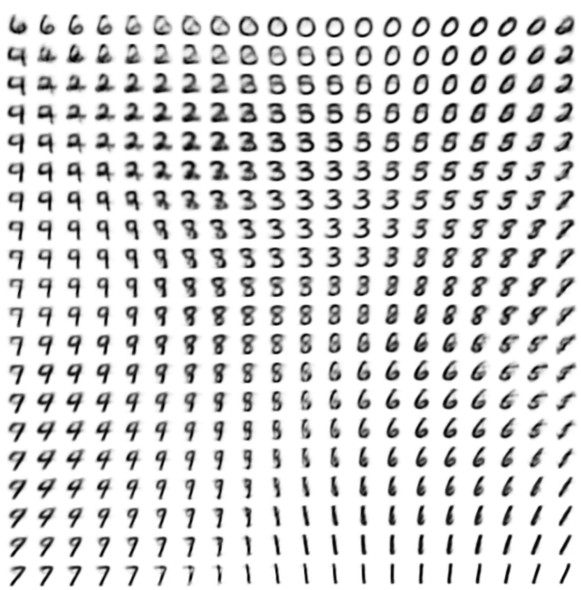
(Erdogan et al., 2016)

Variational Auto-Encoder (VAE)

- Vanilla VAE

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





(Shafkat et al. 2016)

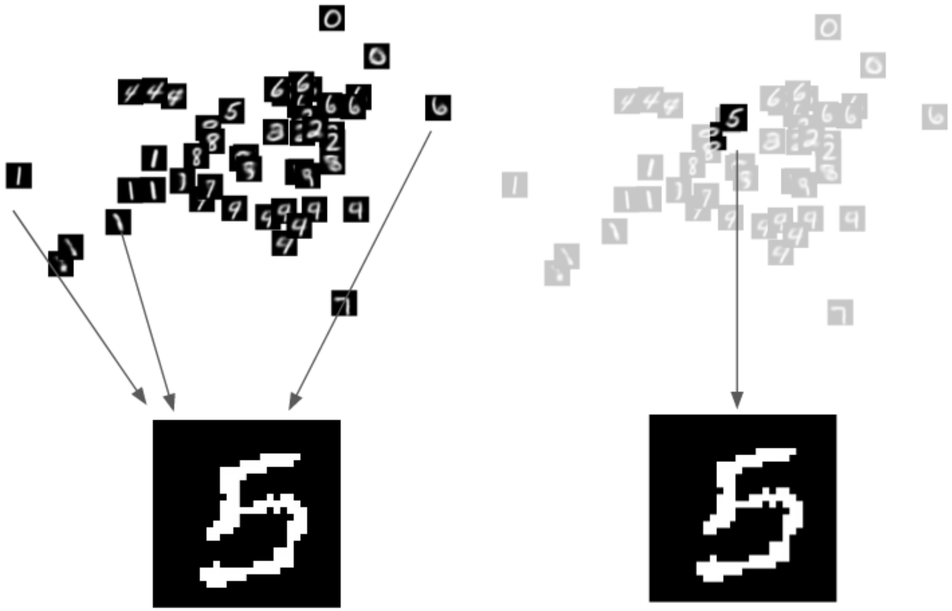
(Kingma et al. 2014)

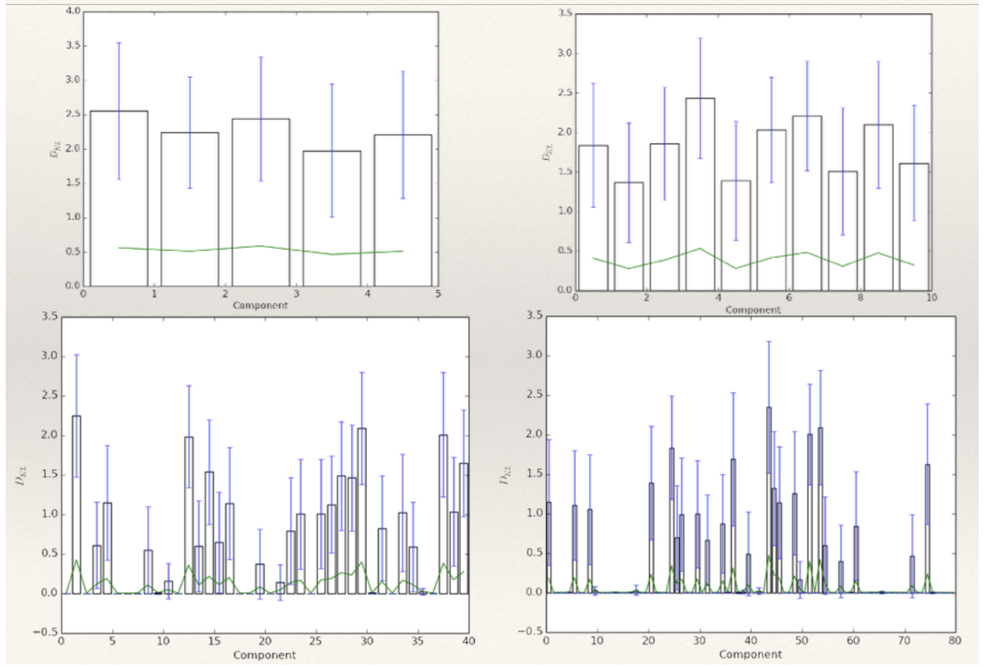
Caveats, Information Theoretic POV

- Regularized Autoencoder?

the smaller the better?

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





(Dinh & Dumoulin 2014)

Evaluation

- Importance Sampling (stochastic lower bound)

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

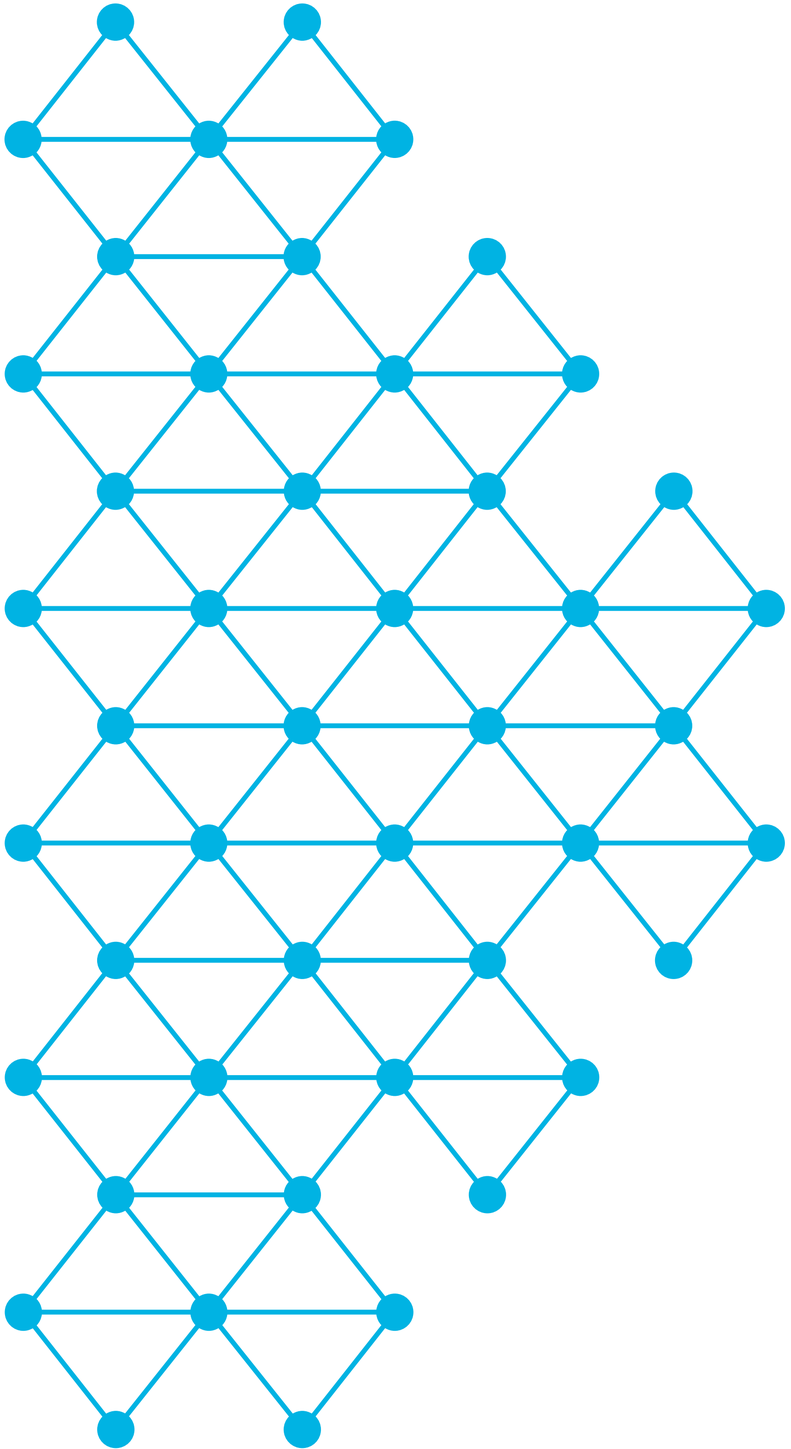
$$\log p(x) \approx \mathrm{L}\overset{M}{\underset{m=1}{\Sigma}}\mathrm{E}\left[\log p(x, z_m) - \log q(z_m|x)\right]$$

- Further reading: Annealed Importance Sampling by Radford Neal

(Neal, 1998)

What Assumptions have we made so far?

- What can we change? (Non-Vanilla VAE)
  - fixing $p(z) = \mathcal{N}(0, \mathrm{I})$
  - 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 $\Phi : \phi \in \Phi$

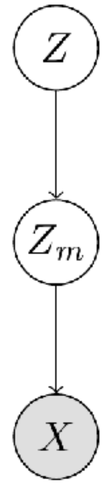


Better Model Assumptions

What likelihood p(x|z) to use?

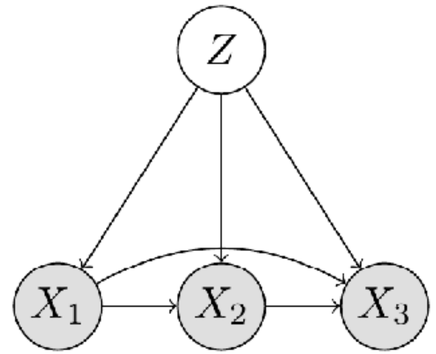
- Hierarchy?

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



- Autoregressive model?

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

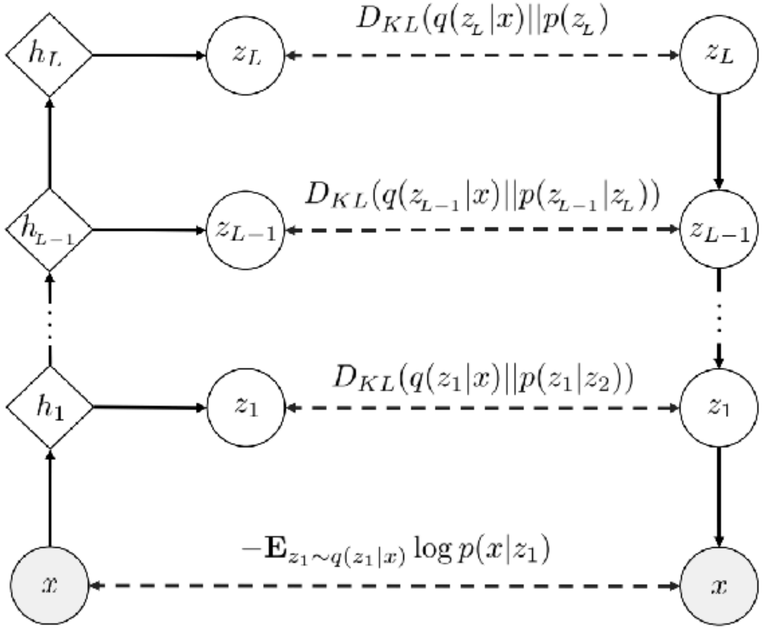


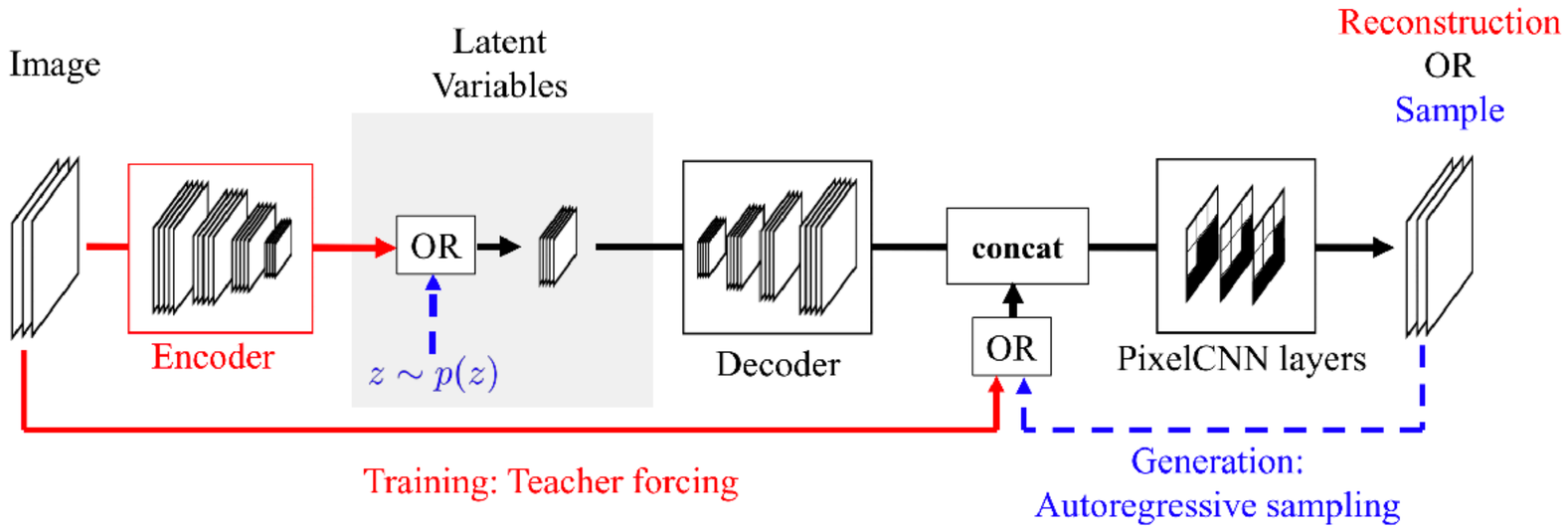
PixelVAE

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

$$\vdots$$

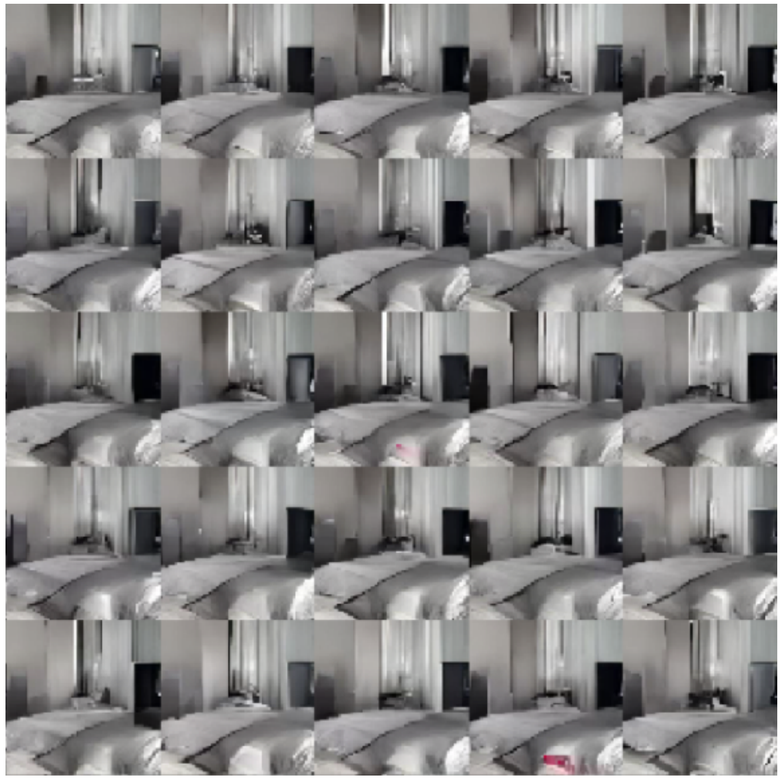
$$= -E_{z_1\sim q(z_1|x)} \log p(x|z_1) + \sum_{i=1}^{L} \mathbf{E}_{z_{i+1}\sim q(z_{i+1}|x)} \left[D_{KL}(q(z_i|x)||p(z_i|z_{i+1})) \right] \qquad p(x|z_1) = \prod_j p(x_j|x_{j'<j}, z_1)$$

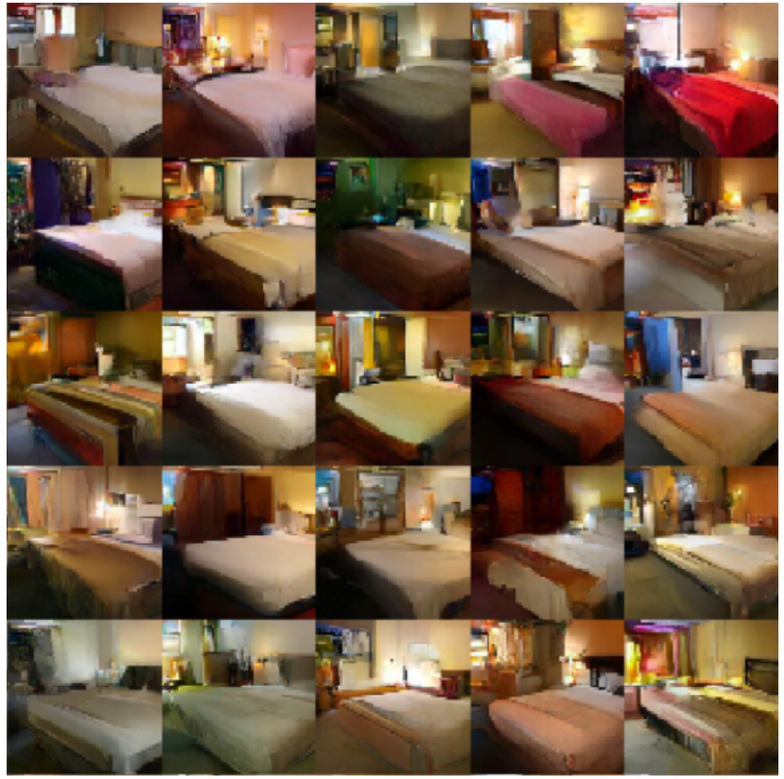




(Gulrajani et al., 2017)

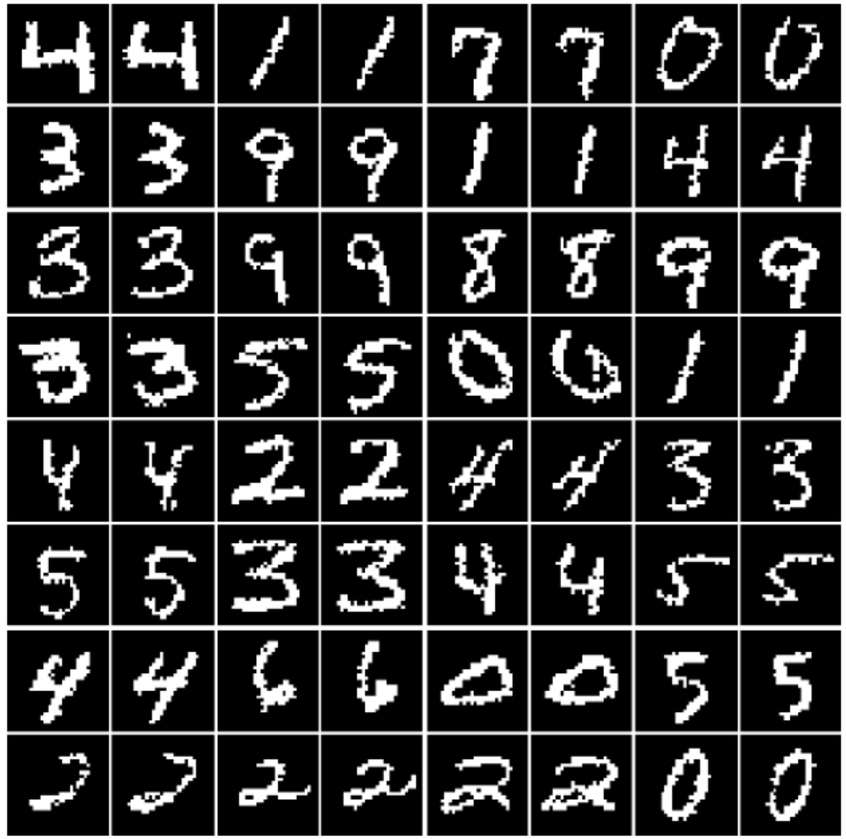
PixelVAE samples

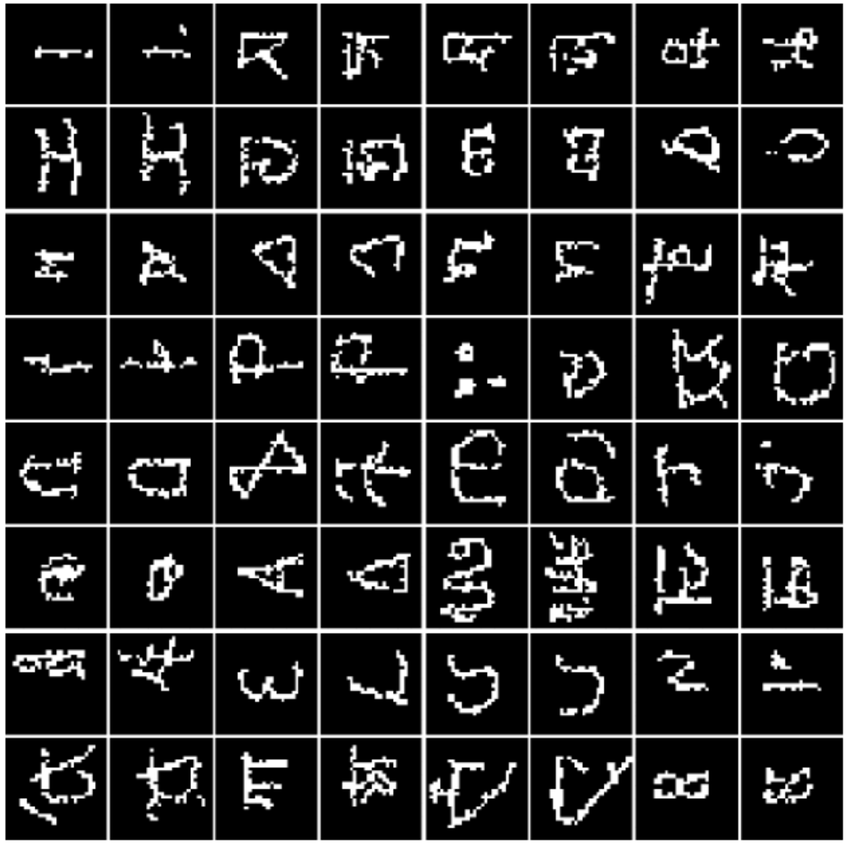




(Gulrajani et al., 2017)

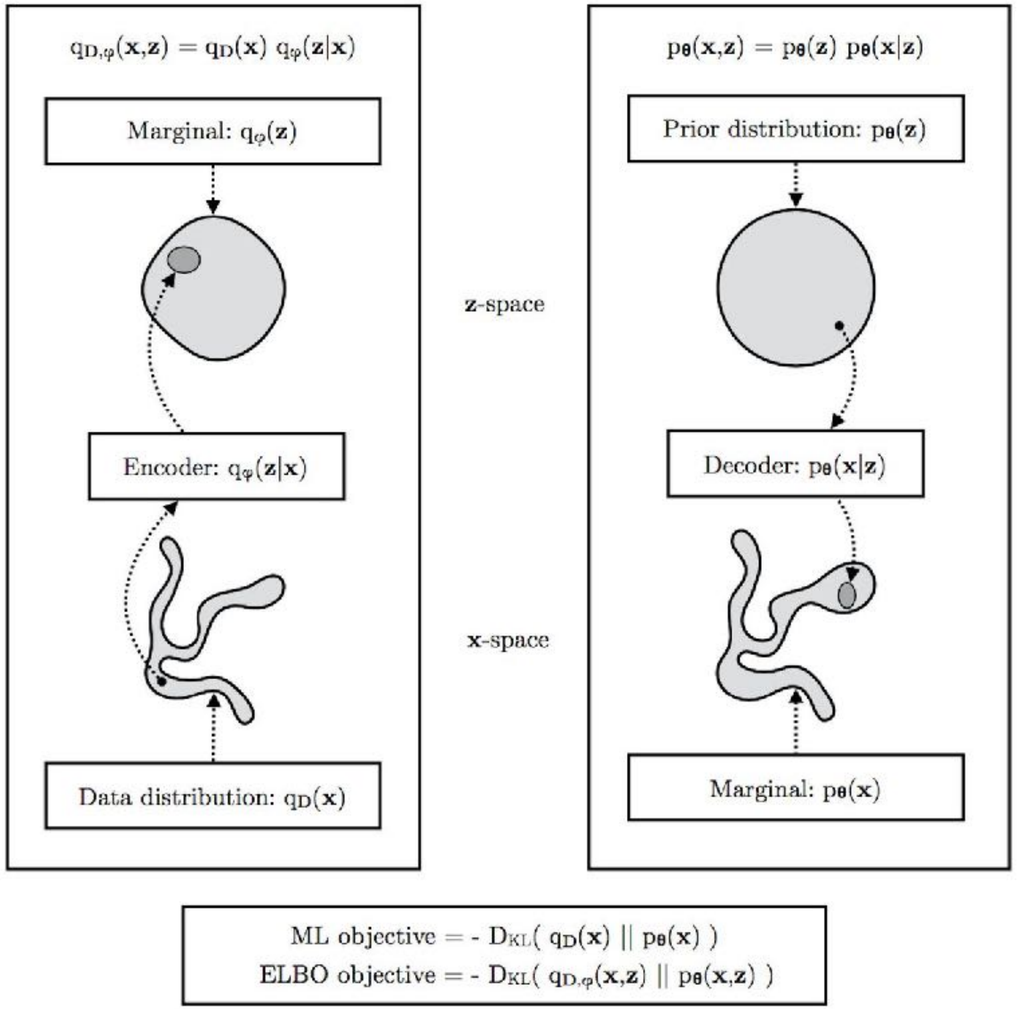
Lossy Encoding





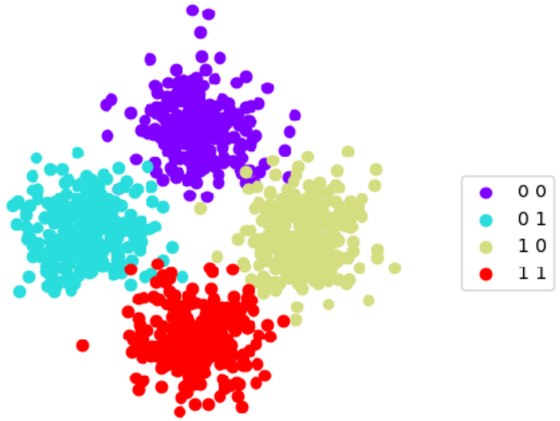
(Chen et al., 2017)

What prior p(z) to use?

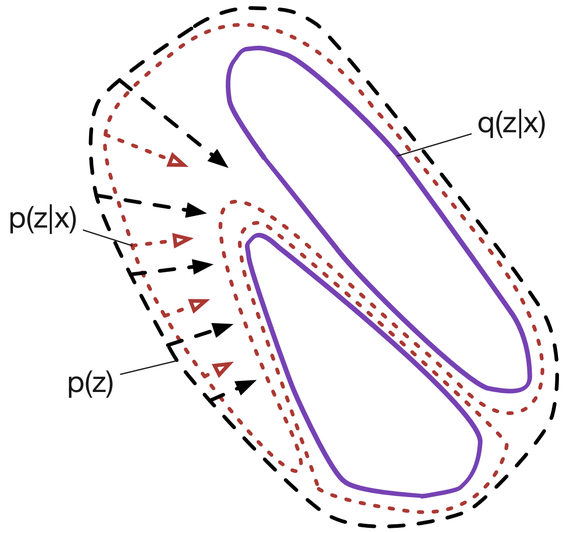


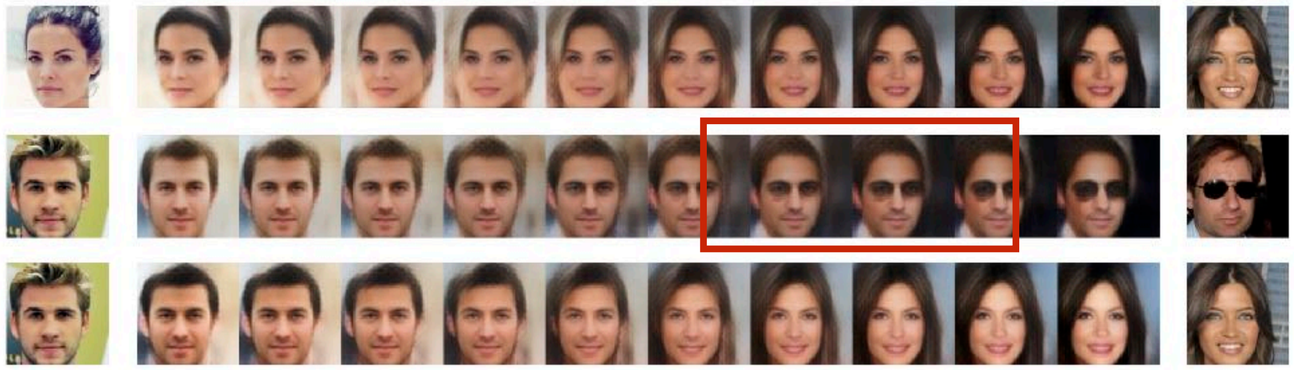
ML objective = - $D_{KL}(\, q_D(\mathbf{x}) \,||\, p_\theta(\mathbf{x})\,)$
ELBO objective = - $D_{KL}(\, q_{D,\varphi}(\mathbf{x},\mathbf{z}) \,||\, p_\theta(\mathbf{x},\mathbf{z})\,)$

(Kingma et al. 2017)



$$q(z) = \sum_x q_{\mathcal{D}}(x) q_\phi(z|x) = \mathbb{E}_{q_{\mathcal{D}}(x)}\left[q(z|x)\right]$$





(Huang et al., 2017; Hou et al., 2016)

Prior Can Be Learned!

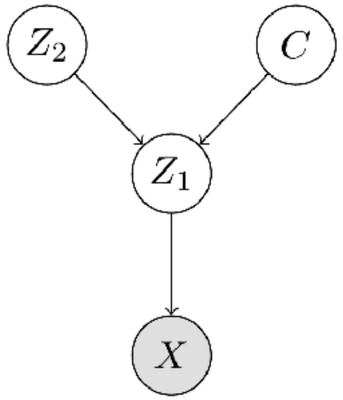
if DLGMs find it difficult to produce unimodal Gaussian marginal posteriors, then perhaps we should investigate multimodal priors that can meet q(z) halfway.

— Matt Hoffman, 2016

NIPS Workshop on Advances in Approximate Bayesian Inference Workshop

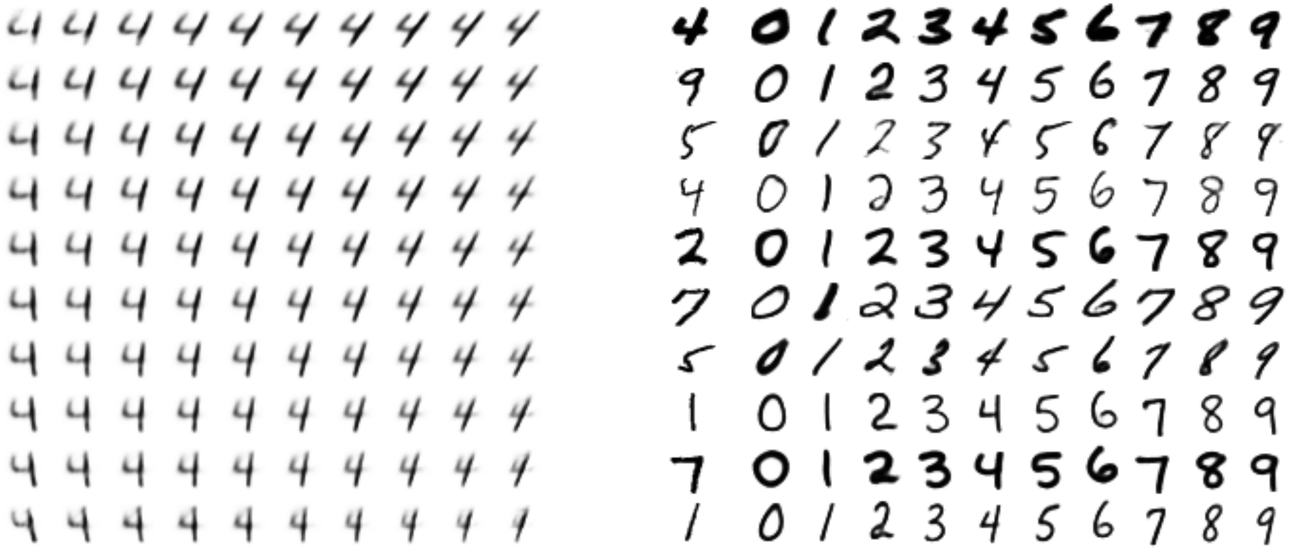
(Hoffman & Johnson, 2016)

Multimodal Prior

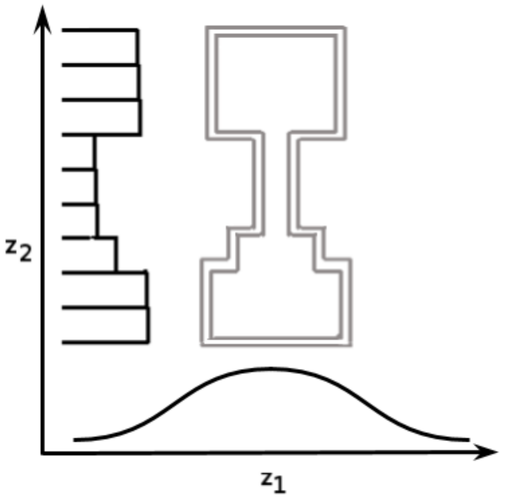


$$p(z_1|z_2) = \sum_c p(z_1|z_2, c)p(c)$$

mixture (of Gaussians) prior



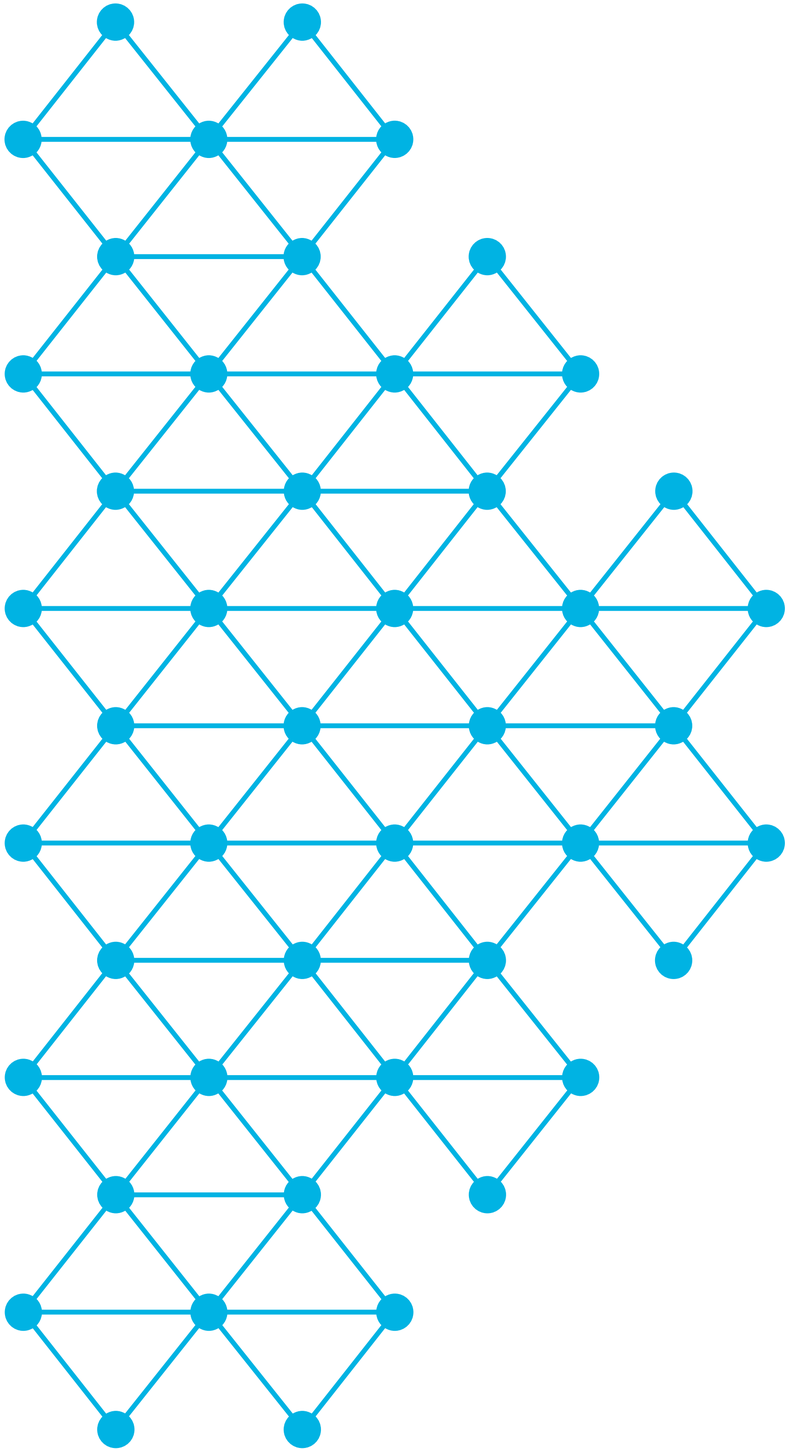
(Kingma et al., 2014; Dilokthanakul et al. 2016)



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

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

(Serban et al., 2016)



Better Inference

Suboptimality in Variational Inference

$$\log p_\theta(x) - \mathcal{L}(\theta, \phi; x) = \underbrace{D_{\mathrm{KL}}\left(q^* \| p\right)}_{\text{Gap 1}} + \underbrace{\left[D_{\mathrm{KL}}\left(q_\theta^* \| p\right) - D_{\mathrm{KL}}\left(q^* \| p\right)\right]}_{\text{Gap 2}} + \underbrace{\left[D_{\mathrm{KL}}\left(q_\theta \| p\right) - D_{\mathrm{KL}}\left(q_\theta^* \| p\right)\right]}_{\text{Gap 3}}$$

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
$\mathcal{L}_{\mathrm{VAE}}[q^*_{Flow}]$	-90.83	-90.05	-90.40	-90.26	-98.03	-95.93	-97.74	-96.87
$\mathcal{L}_{\mathrm{VAE}}[q^*_{FFG}]$	-91.19	-90.34	-102.88	-103.53	-99.03	-98.09	-130.90	-129.24
$\mathcal{L}_{\mathrm{VAE}}[q]$	-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

(Cremer et al. 2017)

(Krishnan et al., 2017; Marino et al., 2017; Kim et al., 2018)

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_ϕ [17]	✗	✗	✗
MCMC on top of q_ϕ [3, 5]	(✗)	(✗)	(✗)
Gradient flow [4]	✗	✗	✗
Importance sampling [1]	(✗)	(✗)	(✗)

Reducing Variational Gap Ref

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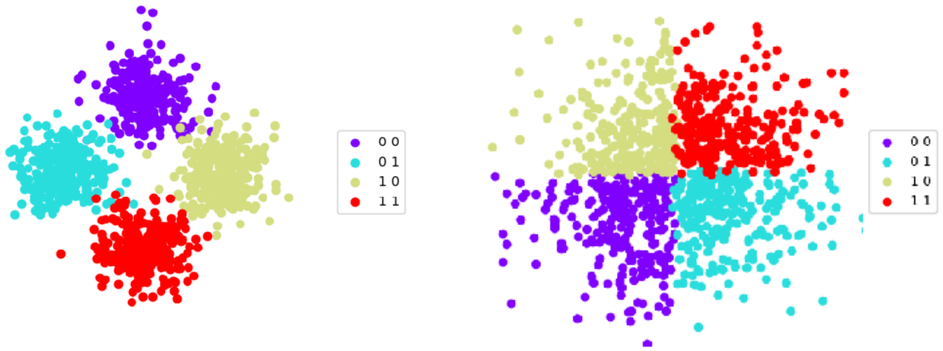
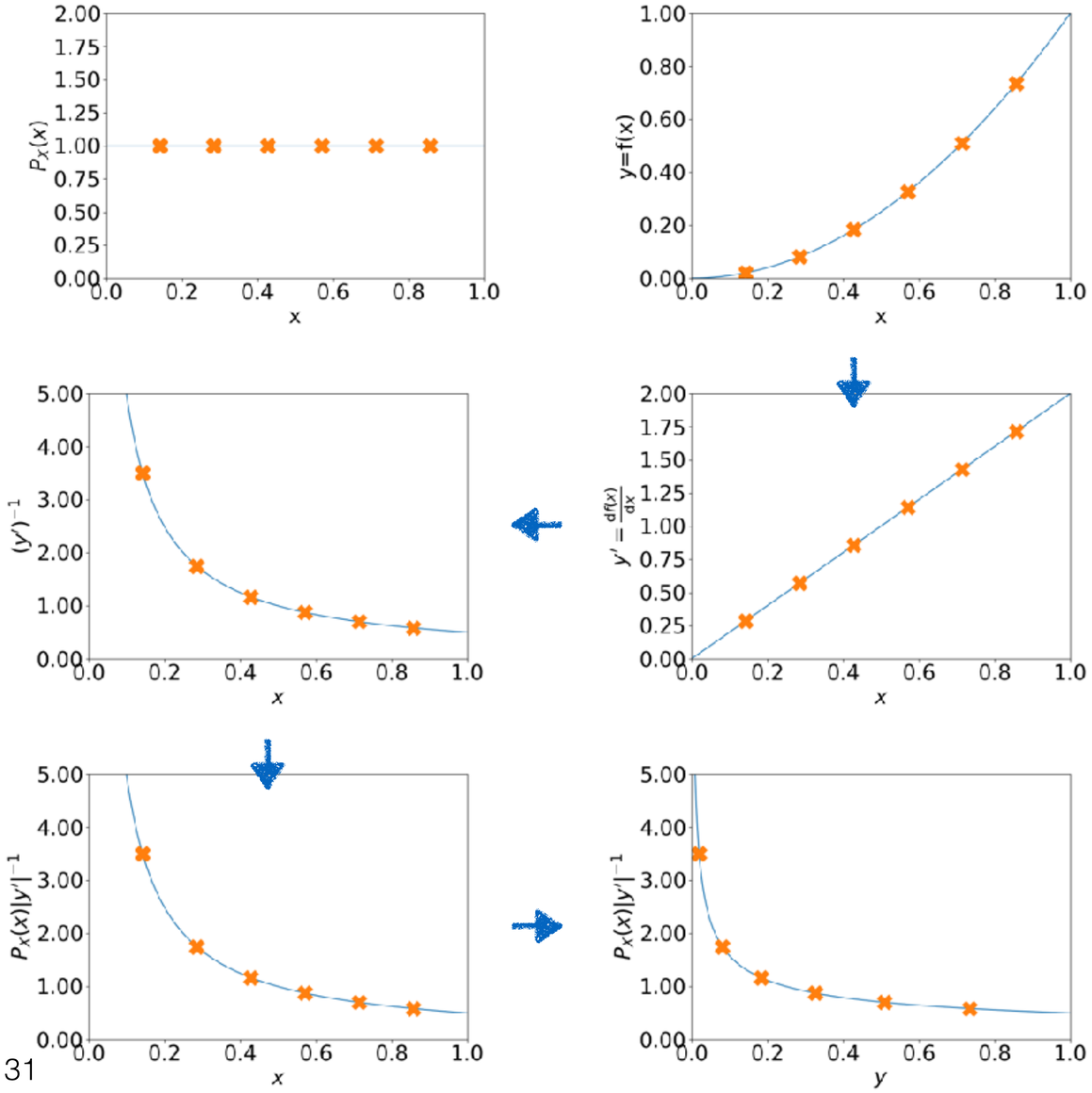
Transformation Methods: Normalizing Flows



- Change of variable distribution

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

$$P_Y(y) = P_X(x) \left| \frac{\mathrm{d}f(x)}{\mathrm{d}x} \right|^{-1}$$



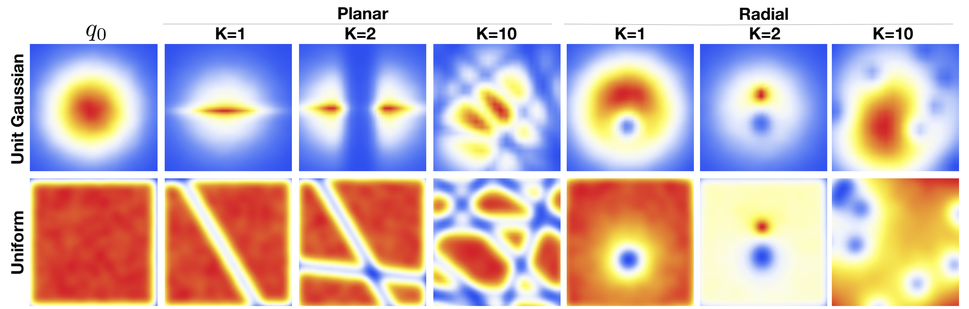
(Rezende & Mohamed 2016)

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

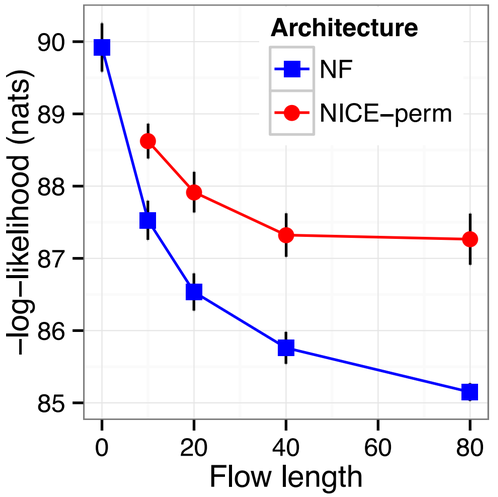
$$z_K = f_K \circ \ldots \circ f_2 \circ f_1(z_0)$$

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



- Law of unconscious statistician (LOTUS)

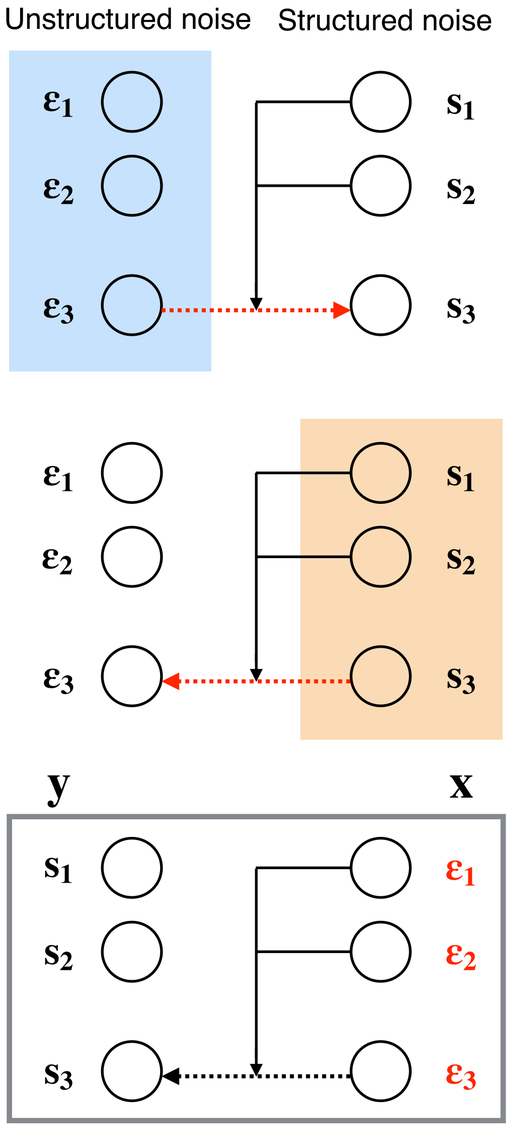
$$\mathbb{E}_{z_K}\left[h(z_K)\right] = \mathbb{E}_{z_0}\left[h(f_K \circ \ldots \circ f_2 \circ f_1(z_0))\right]$$



How to rewrite the ELBO objective?

(Rezende & Mohamed 2016)

Inverse Autoregressive Flows



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

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

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

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

- Change of variable distribution

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

$$P_Y(y) = P_X(x) \left| \frac{\mathrm{d}f(x)}{\mathrm{d}x} \right|^{-1}$$

Autoregressive model

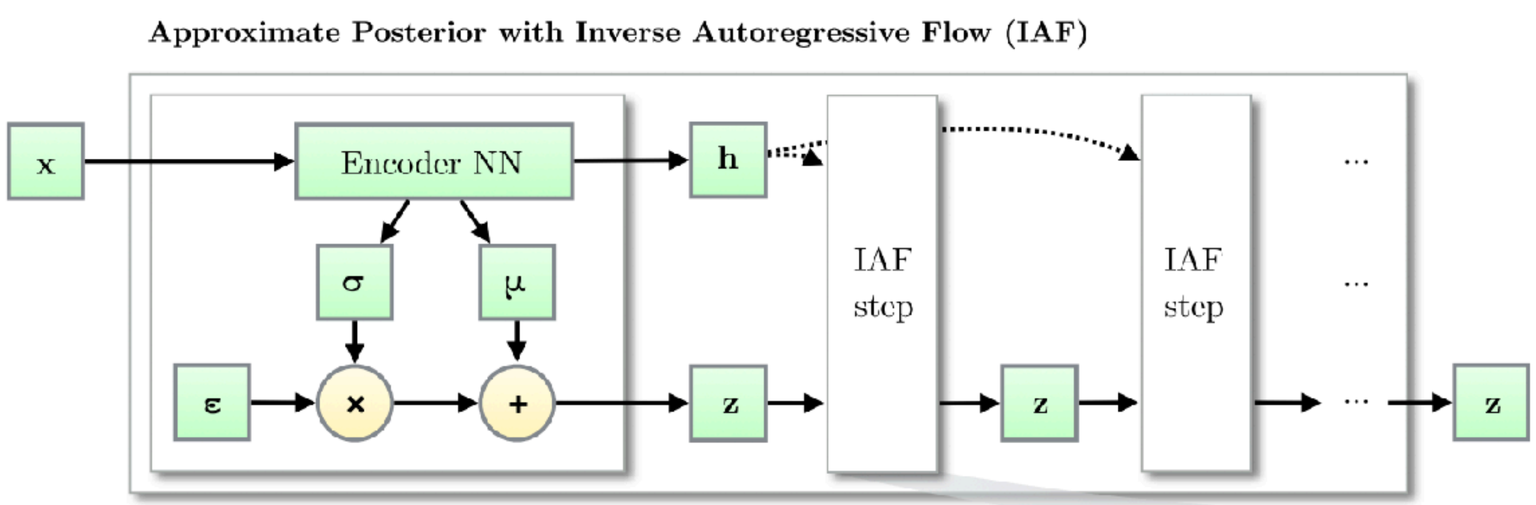
$$p(y_{1:P}) = p(y_1) \prod_{j=2}^{P} p(y_j | y_{1:j-1})$$

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

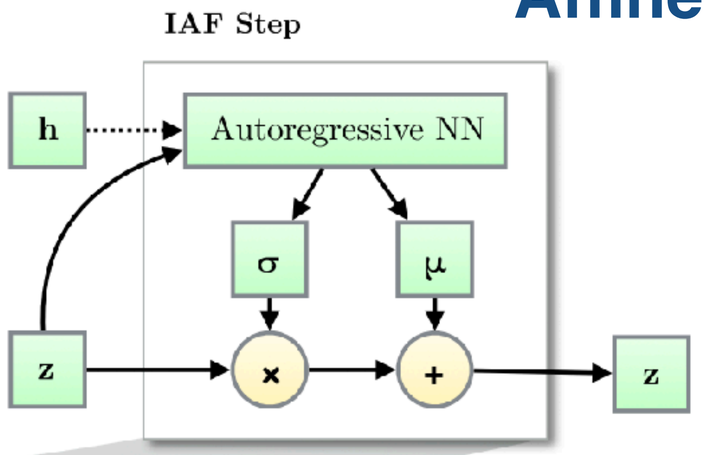
- *Scales well to high-dimensional space in terms of complexity (no rank-one restriction)*
- *Linear complexity in computing log determinant of Jacobian (upper triangular Jacobian)*
- *No dependency in sampling (non-sequential)*
- *More expressive than pure autoregressive model (composable)*

(Kingma et al., 2016; Huang et al., 2018)

Improving Variational Inference with IAF



Affine



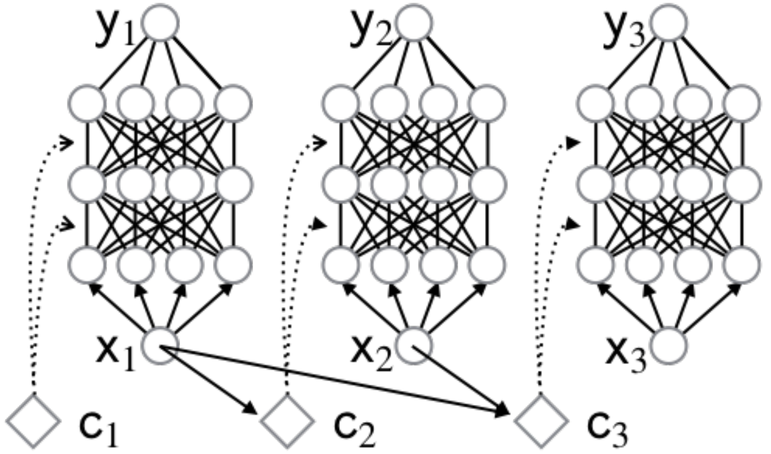
Non-affine

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

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

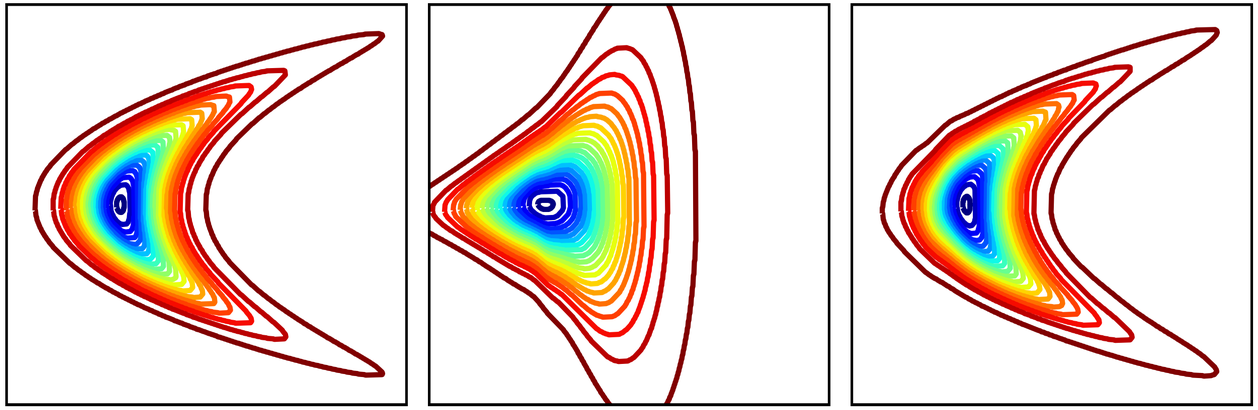
$$z_k = \mu_k(z_{k-1}) + \sigma_k(z_{k-1}) \odot z_{k-1}$$

Method	bits/dim ≤
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)	**3.00**
Gated PixelCNN (van den Oord et al., 2016c)	**3.03**
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)	**3.11**



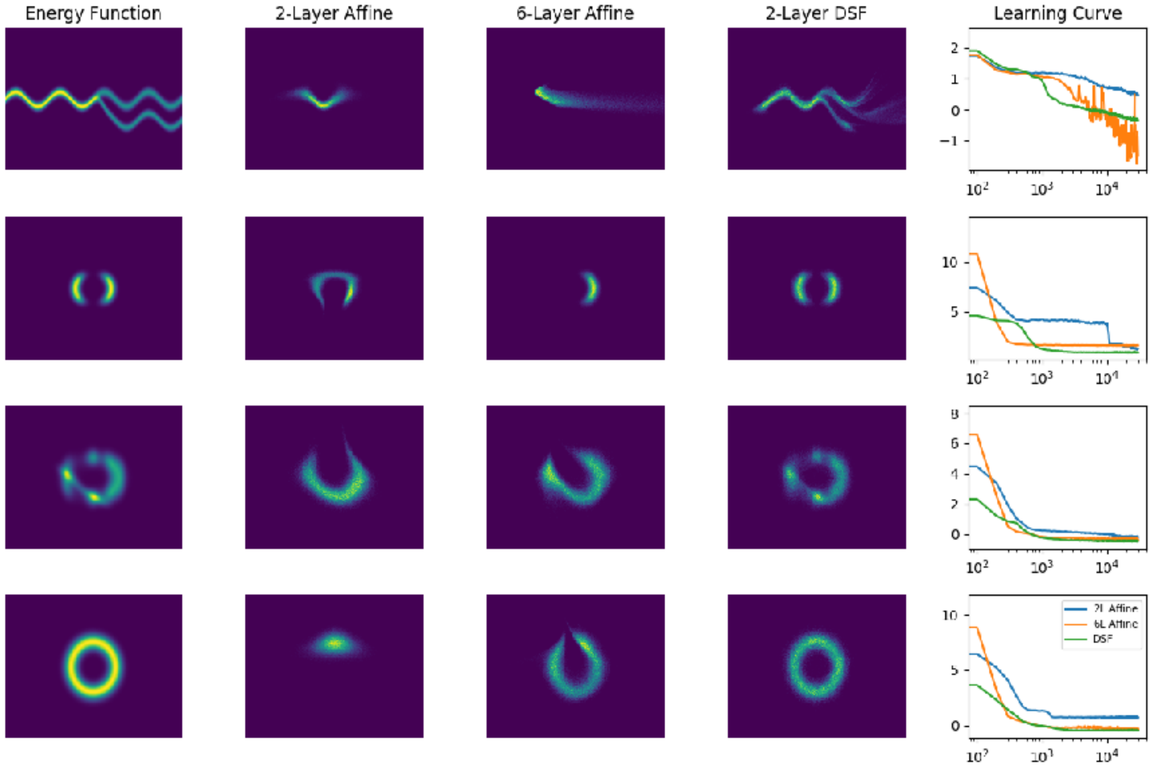
(Kingma et al., 2016; Huang et al., 2018)

Expressiveness of Autoregressive FLows



Target MADE 5 MADEs

(Papamakarios, 2017)



(Huang et al., 2017-(b))

Importance Weighted Autoencoders

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

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

		MNIST			
		VAE		IWAE	
# stoch. layers	k	NLL	active units	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*

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

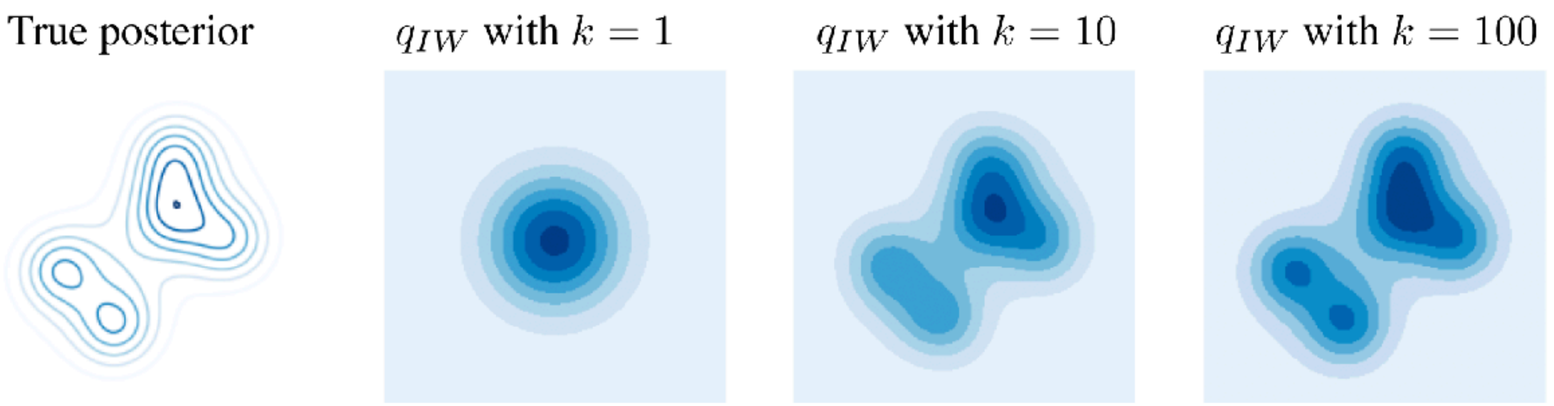
Moreover, if $p(\mathbf{h}, \mathbf{x})/q(\mathbf{h}|\mathbf{x})$ is bounded, then $\mathcal{L}_k$ approaches $\log p(\mathbf{x})$ as k goes to infinity.

(Burda et al. 2016)

Iterative Refinement with Importance Sampling

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

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

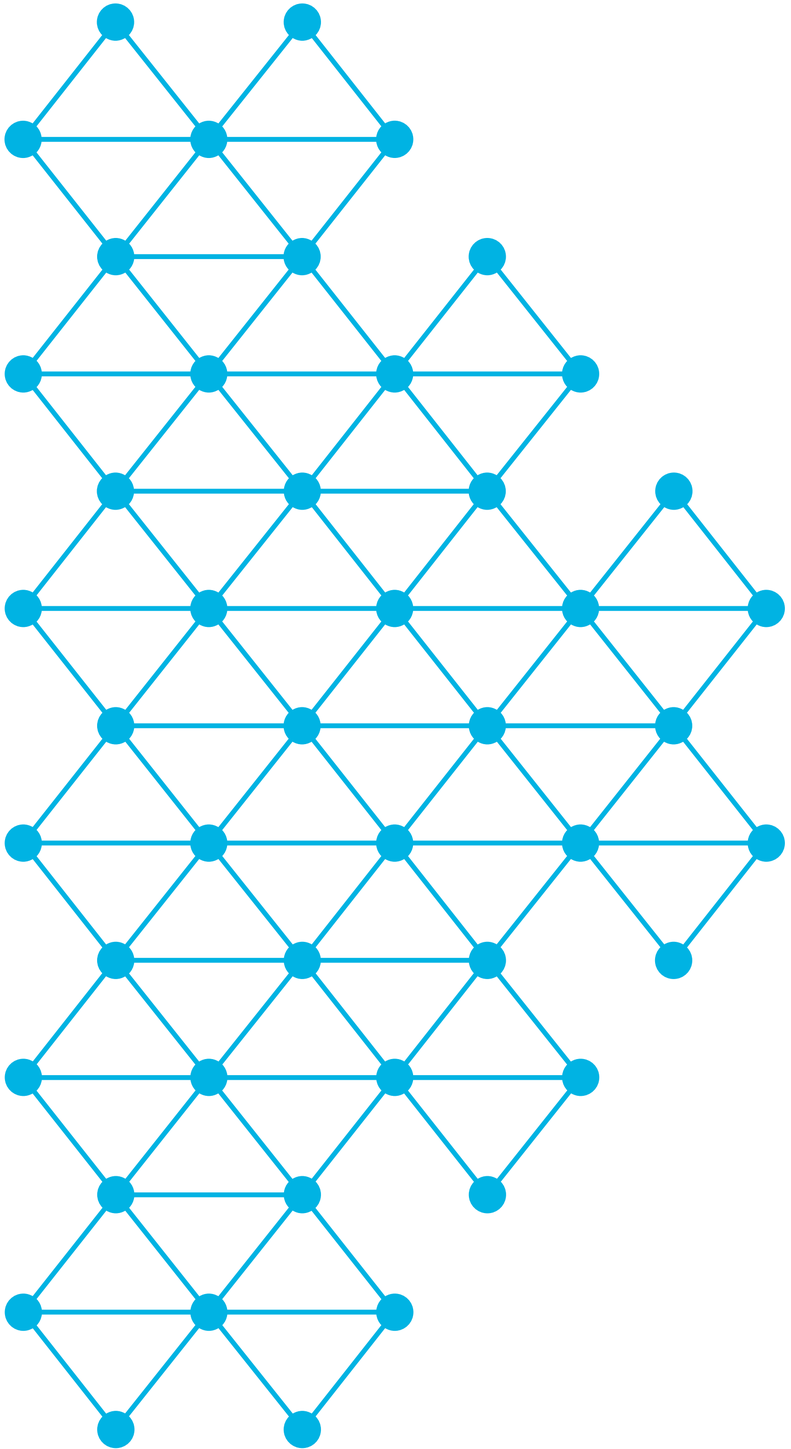


(Cremer et al. 2017-(b))

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



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