

# Deep Generative Models

## Lecture supplementary

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# Outline I

## 1. Autoregressive models

Masked Autoencoder (MADE)  
GatedPixelCNN

## 2. Variational inference

ELBO gradient, Log derivative trick  
Mean field approximation

## 3. VAE-related topics

IWAE  
PixelVAE, Hierarchical VAE  
Posterior collapse

## 4. Normalizing Flows

Flows intuition  
Residual Flows (planar flows)  
Autoregressive flows  
Parallel WaveNet

## 5. RevNet, i-RevNet

## Outline II

6. ELBO surgery

7. Disentanglement

InfoGAN

$\beta$ -VAE

DIP-VAE

FactorVAE

Challenging Disentanglement Assumptions

8. GANs

DCGAN

Improved techniques for training GANs

WGAN

StyleGAN

9. FFJORD

10. Vector Quantized VAE-2

11. Feature Quantized GAN

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## 9. FFJORD

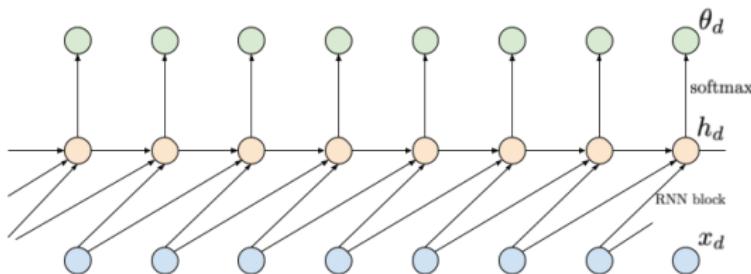
## 10. Vector Quantized VAE-2

## 11. Feature Quantized GAN

## Autoregressive models

- ▶ Previous model has **limited** memory  $d$ . It is insufficient for many modalities (e.g. for images and text).
- ▶ Recurrent NN fixes this problem and potentially could learn long-range dependencies:

$$p(x_j | \mathbf{x}_{1:j-1}, \theta) = p(x_j | \mathbf{h}_j, \theta), \quad \mathbf{h}_j = \text{RNN}(\mathbf{x}_{j-d:j-1}, \mathbf{h}_{j-1})$$



- ▶ Sequential computation of all conditionals  $p(x_j | \mathbf{x}_{1:j-1}, \theta)$ , hence, the training is slow.
- ▶ RNN suffers from vanishing and exploding gradients.

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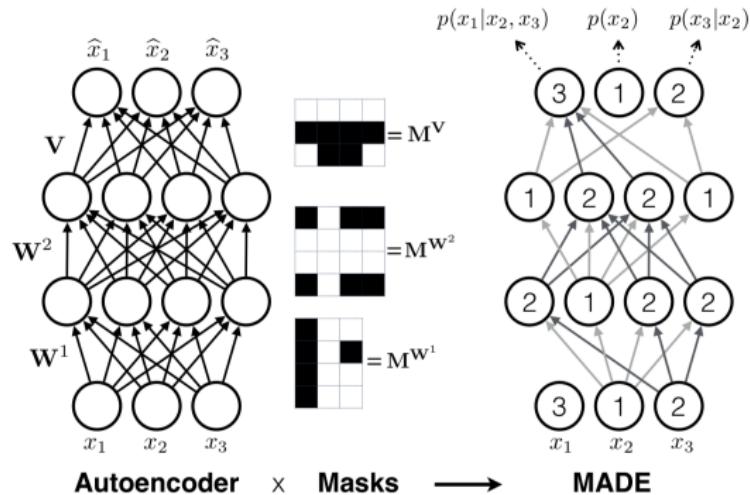
## 9. FFJORD

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# MADE

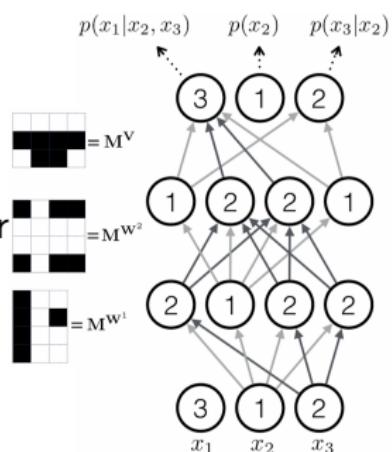
- ▶ Vanila autoencoder is not a generative model.
- ▶ Let mask the weight matrices to make the model generative:  
 $\mathbf{W}_M = \mathbf{W} \cdot \mathbf{M}$ .



- ▶ The question is how to create matrices  $\mathbf{M}$  which produce the autoregressive property?

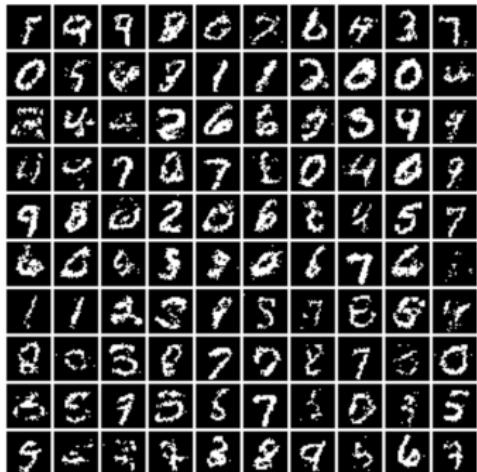
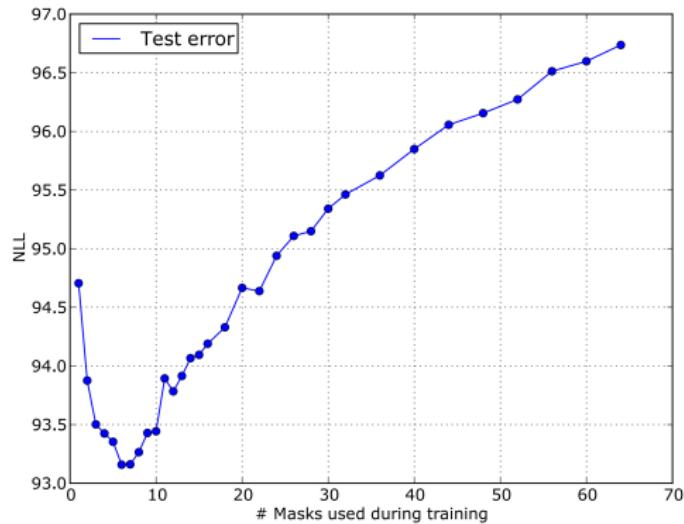
## Masks generation

- ▶ Define the ordering of input elements from 1 to  $m$ .
- ▶ Assign the random number  $k$  from 1 to  $m - 1$  to each hidden unit. The number gives the maximum value of input units to which the unit can be connected.
- ▶ Connect each hidden unit with number  $k$  with the previous layer units which has the number is **less or equal** than  $k$ .
- ▶ Connect each output unit with number  $k$  with the previous layer units which has the number is **less** than  $k$ .



## Possible variations

- ▶ Order agnostic training (missing values in partially observed input vectors can be imputed efficiently);
- ▶ Connectivity-agnostic training (cheap ensembling).



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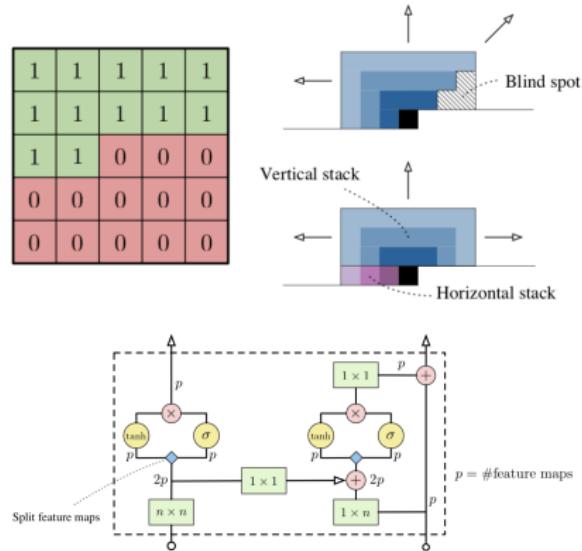
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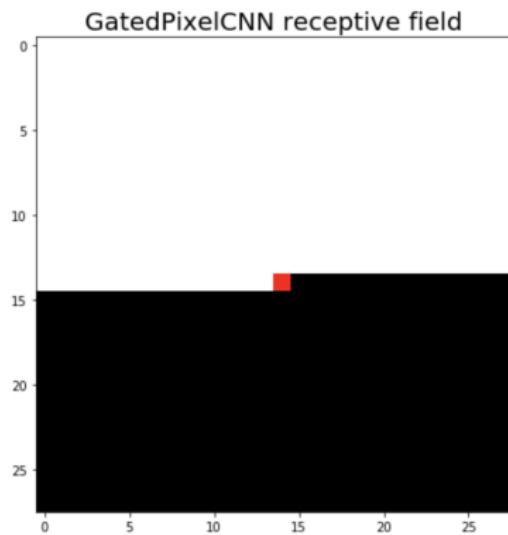
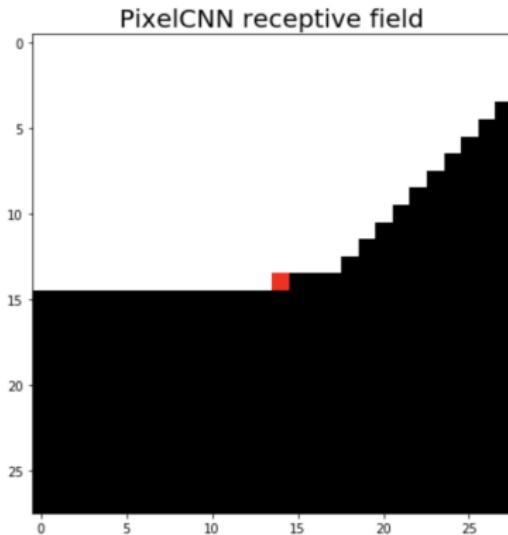
# GatedPixelCNN (2016)



Van den Oord A. et al. Conditional image generation with pixelcnn decoders

<https://arxiv.org/pdf/1606.05328.pdf>

# GatedPixelCNN (2016)



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Van den Oord A. et al. Conditional image generation with pixelcnn decoders  
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## Extensions

- ▶ **PixelCNN++**: *Improving the PixelCNN with Discretized Logistic Mixture Likelihood and Other Modifications*  
<https://arxiv.org/pdf/1701.05517.pdf>  
(mixture of logistics instead of softmax);
- ▶ **PixelSNAIL**: *An Improved Autoregressive Generative Model*  
<https://arxiv.org/pdf/1712.09763.pdf>  
(self-attention to learn optimal autoregression ordering).

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## ELBO gradient (E-step, $\nabla_{\phi}\mathcal{L}(\phi, \theta)$ )

$$\mathcal{L}(\phi, \theta) = \mathbb{E}_q \log p(\mathbf{X}|\mathbf{Z}, \theta) - KL(q(\mathbf{Z}|\mathbf{X}, \phi) || p(\mathbf{Z})) \rightarrow \max_{\phi, \theta} .$$

Difference from M-step: density function  $q(\mathbf{z}|\mathbf{x}, \phi)$  depends on the parameters  $\phi$ , it is impossible to use Monte-Carlo estimation:

$$\nabla_{\phi}\mathcal{L}(\phi, \theta) = \int \nabla_{\phi} q(\mathbf{Z}|\mathbf{X}, \phi) \log p(\mathbf{X}|\mathbf{Z}, \theta) d\mathbf{Z} - \nabla_{\phi} KL$$

### Log-derivative trick

$$\nabla_{\xi} q(\eta|\xi) = q(\eta|\xi) \left( \frac{\nabla_{\xi} q(\eta|\xi)}{q(\eta|\xi)} \right) = q(\eta|\xi) \nabla_{\xi} \log q(\eta|\xi).$$

$$\nabla_{\phi} q(\mathbf{Z}|\mathbf{X}, \phi) = q(\mathbf{Z}|\mathbf{X}, \phi) \nabla_{\phi} \log q(\mathbf{Z}|\mathbf{X}, \phi).$$

## ELBO gradient (E-step, $\nabla_{\phi}\mathcal{L}(\phi, \theta)$ )

$$\begin{aligned}\nabla_{\phi}\mathcal{L}(\phi, \theta) &= \int \nabla_{\phi}q(\mathbf{Z}|\mathbf{X}, \phi) \log p(\mathbf{X}|\mathbf{Z}, \theta) d\mathbf{Z} - \nabla_{\phi}KL = \\ &= \int q(\mathbf{Z}|\mathbf{X}, \phi) [\nabla_{\phi} \log q(\mathbf{Z}|\mathbf{X}, \phi) \log p(\mathbf{X}|\mathbf{Z}, \theta)] d\mathbf{Z} - \nabla_{\phi}KL\end{aligned}$$

After applying log-reparametrization trick, we are able to use Monte-Carlo estimation:

$$\begin{aligned}\nabla_{\phi}\mathcal{L}(\phi, \theta) &\approx n \nabla_{\phi} \log q(\mathbf{z}_i^* | \mathbf{x}_i, \phi) \log p(\mathbf{x}_i | \mathbf{z}_i^*, \theta) - \nabla_{\phi}KL, \\ \mathbf{z}_i^* &\sim q(\mathbf{z}_i | \mathbf{x}_i, \phi).\end{aligned}$$

### Problem

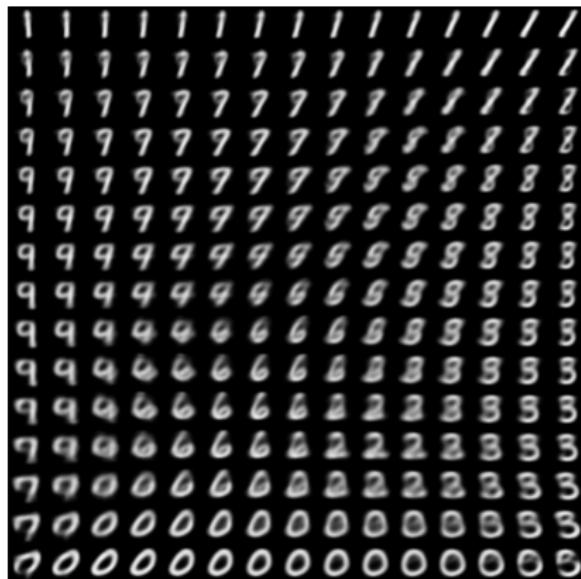
Unstable solution with huge variance.

### Solution

Reparametrization trick

# Variational Autoencoder

Generated images for latent objects  $\mathbf{z}$  sampled from prior  $\mathcal{N}(0, \mathbf{I})$



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## VAE as Bayesian model

Posterior distribution

$$p(\theta|\mathbf{X}) = \frac{p(\mathbf{X}|\theta)p(\theta)}{p(\mathbf{X})}$$

ELBO

$$\begin{aligned}\log p(\theta|\mathbf{X}) &= \log p(\mathbf{X}|\theta) + \log p(\theta) - \log p(\mathbf{X}) \\ &= \mathcal{L}(q, \theta) + KL(q||p) + \log p(\theta) - \log p(\mathbf{X}) \\ &\geq [\mathcal{L}(q, \theta) + \log p(\theta)] - \log p(\mathbf{X}).\end{aligned}$$

EM-algorithm

► E-step

$$q(\mathbf{z}) = \arg \max_q \mathcal{L}(q, \theta^*) = \arg \min_q KL(q||p) = p(\mathbf{z}|\mathbf{x}, \theta^*);$$

► M-step

$$\theta^* = \arg \max_{\theta} [\mathcal{L}(q, \theta) + \log p(\theta)].$$

# Bayesian framework

## Bayes theorem

$$p(\mathbf{t}|\mathbf{x}) = \frac{p(\mathbf{x}|\mathbf{t})p(\mathbf{t})}{p(\mathbf{x})} = \frac{p(\mathbf{x}|\mathbf{t})p(\mathbf{t})}{\int p(\mathbf{x}|\mathbf{t})p(\mathbf{t})d\mathbf{t}}$$

- ▶  $\mathbf{x}$  – observed variables,  $\mathbf{t}$  – unobserved variables (latent variables/parameters);
- ▶  $p(\mathbf{x}|\mathbf{t})$  – likelihood;
- ▶  $p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{t})p(\mathbf{t})d\mathbf{t}$  – evidence;
- ▶  $p(\mathbf{t})$  – prior distribution,  $p(\mathbf{t}|\mathbf{x})$  – posterior distribution.

## Meaning

We have unobserved variables  $\mathbf{t}$  and some prior knowledge about them  $p(\mathbf{t})$ . Then, the data  $\mathbf{x}$  has been observed. Posterior distribution  $p(\mathbf{t}|\mathbf{x})$  summarizes the knowledge after the observations.

## Variational Lower Bound

We have set of objects  $\mathbf{X} = \{\mathbf{x}_i\}_{i=1}^n$ . The goal is to perform Bayesian inference on the unobserved variables  $\mathbf{T} = \{\mathbf{t}_i\}_{i=1}^n$ .

### Evidence Lower Bound (ELBO)

$$\begin{aligned}\log p(\mathbf{X}) &= \log \frac{p(\mathbf{X}, \mathbf{T})}{p(\mathbf{T}|\mathbf{X})} = \\&= \int q(\mathbf{T}) \log \frac{p(\mathbf{X}, \mathbf{T})}{p(\mathbf{T}|\mathbf{X})} d\mathbf{T} = \int q(\mathbf{T}) \log \frac{p(\mathbf{X}, \mathbf{T})q(\mathbf{T})}{p(\mathbf{T}|\mathbf{X})q(\mathbf{T})} d\mathbf{T} = \\&= \int q(\mathbf{T}) \log \frac{p(\mathbf{X}, \mathbf{T})}{q(\mathbf{T})} d\mathbf{T} + \int q(\mathbf{T}) \log \frac{q(\mathbf{T})}{p(\mathbf{T}|\mathbf{X})} d\mathbf{T} = \\&= \mathcal{L}(q) + KL(q(\mathbf{T})||p(\mathbf{T}|\mathbf{X})) \geq \mathcal{L}(q).\end{aligned}$$

We would like to maximize lower bound  $\mathcal{L}(q)$ .

## Mean field approximation

### Independence assumption

$$q(\mathbf{T}) = \prod_{i=1}^k q_i(\mathbf{T}_i), \quad \mathbf{T} = [\mathbf{T}_1, \dots, \mathbf{T}_k], \quad \mathbf{T}_j = \{\mathbf{t}_{ij}\}_{i=1}^n, \quad \mathbf{t}_i = \{\mathbf{T}_{ij}\}_{j=1}^k.$$

Block coordinate optimization of ELBO for  $q_j(\mathbf{T}_j)$

$$\begin{aligned} \mathcal{L}(q) &= \int q(\mathbf{T}) \log \frac{p(\mathbf{X}, \mathbf{T})}{q(\mathbf{T})} d\mathbf{T} = \int \left[ \prod_{i=1}^k q_i(\mathbf{T}_i) \right] \log \frac{p(\mathbf{X}, \mathbf{T})}{\left[ \prod_{i=1}^k q_i(\mathbf{T}_i) \right]} \prod_{i=1}^k d\mathbf{T}_i = \\ &= \int \left[ \prod_{i=1}^k q_i \right] \log p(\mathbf{X}, \mathbf{T}) \prod_{i=1}^k d\mathbf{T}_i - \sum_{i=1}^k \int \left[ \prod_{j=1}^k q_j \right] \log q_i \prod_{j=1}^k d\mathbf{T}_j = \\ &= \int q_j \left[ \int \log p(\mathbf{X}, \mathbf{T}) \prod_{i \neq j} q_i d\mathbf{T}_i \right] d\mathbf{T}_j - \\ &\quad - \int q_j \log q_j d\mathbf{T}_j + \text{const}(q_j) \rightarrow \max_{q_j} \end{aligned}$$

## Mean field approximation

Block coordinate optimization of ELBO for  $q_j(\mathbf{T}_j)$

$$\begin{aligned}\mathcal{L}(q) &= \int q_j \left[ \int \log p(\mathbf{X}, \mathbf{T}) \prod_{i \neq j} q_i d\mathbf{T}_i \right] d\mathbf{T}_j - \int q_j \log q_j d\mathbf{T}_j + \text{const}(q_j) = \\ &= \int q_j \log \hat{p}(\mathbf{X}, \mathbf{T}_j) d\mathbf{T}_j - \int q_j \log q_j d\mathbf{T}_j + \text{const}(q_j) \rightarrow \max_{q_j}.\end{aligned}$$

Here we introduce

$$\log \hat{p}(\mathbf{X}, \mathbf{T}_j) = \int \log p(\mathbf{X}, \mathbf{T}) \prod_{i \neq j} q_i d\mathbf{T}_i = \mathbb{E}_{i \neq j} \log p(\mathbf{X}, \mathbf{T}) + \text{const}(q_j)$$

Final ELBO derivation for  $q_j(\mathbf{T}_j)$

$$\begin{aligned}\mathcal{L}(q) &= \int q_j(\mathbf{T}_j) \log \hat{p}(\mathbf{X}, \mathbf{T}_j) d\mathbf{T}_j - \int q_j(\mathbf{T}_j) \log q_j(\mathbf{T}_j) d\mathbf{T}_j + \text{const}(q_j) = \\ &\quad \int q_j(\mathbf{T}_j) \log \frac{\hat{p}(\mathbf{X}, \mathbf{T}_j)}{q_j(\mathbf{T}_j)} d\mathbf{T}_j + \text{const}(q_j) = \\ &= -KL(q_j(\mathbf{T}_j) || \hat{p}(\mathbf{X}, \mathbf{T}_j)) + \text{const}(q_j) \rightarrow \max_{q_j}.\end{aligned}$$

## Mean field approximation

Independence assumption

$$q(\mathbf{T}) = \prod_{i=1}^k q_i(\mathbf{T}_i), \quad \mathbf{T} = [\mathbf{T}_1, \dots, \mathbf{T}_k], \quad \mathbf{T}_j = \{\mathbf{t}_{ij}\}_{i=1}^n.$$

ELBO

$$\mathcal{L}(q) = -KL(q_j(\mathbf{T}_j) || \hat{p}(\mathbf{X}, \mathbf{T}_j)) + \text{const}(q_j) \rightarrow \max_{q_j}.$$

Solution

$$q_j(\mathbf{T}_j) = \text{const} \cdot \hat{p}(\mathbf{X}, \mathbf{T}_j)$$

$$\log \hat{p}(\mathbf{X}, \mathbf{T}_j) = \mathbb{E}_{i \neq j} \log p(\mathbf{X}, \mathbf{T}) + \text{const}$$

$$\log q_j(\mathbf{T}_j) = \mathbb{E}_{i \neq j} \log p(\mathbf{X}, \mathbf{T}) + \text{const}$$

# Mean field approximation

## ELBO

$$\mathcal{L}(q) = -KL(q_j(\mathbf{T}_j) || \hat{p}(\mathbf{X}, \mathbf{T}_j)) + \text{const}(q_j) \rightarrow \max_{q_j}.$$

## Solution

$$\log q_j(\mathbf{T}_j) = \mathbb{E}_{i \neq j} \log p(\mathbf{X}, \mathbf{T}) + \text{const}$$

Assumptions:

- ▶  $\mathbf{T} = [\mathbf{T}_1, \mathbf{T}_2] = [\mathbf{Z}, \boldsymbol{\theta}]$ ,  $q(\mathbf{T}) = q(\mathbf{T}_1) \cdot q(\mathbf{T}_2) = q(\mathbf{Z}) \cdot q(\boldsymbol{\theta})$ .
- ▶ restrict a class of probability distributions for  $\boldsymbol{\theta}$  to Dirac delta functions:

$$q_2 = q(\mathbf{T}_2) = q(\boldsymbol{\theta}) = \delta(\boldsymbol{\theta} - \boldsymbol{\theta}^*).$$

Under the restrictions the exact solution for  $q_2$  is not reached ( $KL$  can be greater than 0).

## Mean field approximation

General solution

$$\log q_j(\mathbf{T}_j) = \mathbb{E}_{i \neq j} \log p(\mathbf{X}, \mathbf{T}) + \text{const}$$

Solution for  $q_1 = q(\mathbf{Z})$

$$\begin{aligned}\log q(\mathbf{Z}) &= \int q(\boldsymbol{\theta}) \log p(\mathbf{X}, \mathbf{Z}, \boldsymbol{\theta}) d\boldsymbol{\theta} + \text{const} = \\ &= \int \delta(\boldsymbol{\theta} - \boldsymbol{\theta}^*) \log p(\mathbf{X}, \mathbf{Z}, \boldsymbol{\theta}) d\boldsymbol{\theta} + \text{const} = \\ &= \log p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^*) + \text{const.}\end{aligned}$$

EM-algorithm (E-step)

$$q(\mathbf{Z}) = \arg \max_q \mathcal{L}(q, \boldsymbol{\theta}^*) = \arg \min_q KL(q||p) = p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^*).$$

## Mean field approximation

### ELBO

$$\mathcal{L}(q) = -KL(q_j(\mathbf{T}_j) || \hat{p}(\mathbf{X}, \mathbf{T}_j)) + \text{const}(q_j) \rightarrow \max_{q_j}.$$

ELBO maximization w.r.t.  $q_2 = q(\boldsymbol{\theta}) = \delta(\boldsymbol{\theta} - \boldsymbol{\theta}^*)$

$$\begin{aligned}\mathcal{L}(q_1, q_2) &= -KL(q(\boldsymbol{\theta}) || \hat{p}(\mathbf{X}, \boldsymbol{\theta})) + \text{const}(\boldsymbol{\theta}^*) \\ &= \int q(\boldsymbol{\theta}) \log \frac{\hat{p}(\mathbf{X}, \boldsymbol{\theta})}{q(\boldsymbol{\theta})} d\boldsymbol{\theta} + \text{const}(\boldsymbol{\theta}^*) \\ &= \int q(\boldsymbol{\theta}) \log \hat{p}(\mathbf{X}, \boldsymbol{\theta}) d\boldsymbol{\theta} - \int q(\boldsymbol{\theta}) \log q(\boldsymbol{\theta}) d\boldsymbol{\theta} + \text{const}(\boldsymbol{\theta}^*) \\ &= \int \delta(\boldsymbol{\theta} - \boldsymbol{\theta}^*) \log \hat{p}(\mathbf{X}, \boldsymbol{\theta}) d\boldsymbol{\theta} + \text{const}(\boldsymbol{\theta}^*) \rightarrow \max_{\boldsymbol{\theta}^*}\end{aligned}$$

## Mean field approximation

ELBO maximization w.r.t.  $q_2 = q(\theta) = \delta(\theta - \theta^*)$

$$\begin{aligned}\mathcal{L}(q_1, q_2) &= \int \delta(\theta - \theta^*) \log \hat{p}(\mathbf{X}, \theta) d\theta + \text{const} = \log \hat{p}(\mathbf{X}, \theta^*) + \text{const} \\ &= \mathbb{E}_{i \neq j} \log p(\mathbf{X}, \mathbf{T}) + \text{const} = \mathbb{E}_{q_1} \log p(\mathbf{X}, \mathbf{Z}, \theta^*) + \text{const} \\ &= \int q(\mathbf{Z}) \log p(\mathbf{X}, \mathbf{Z} | \theta^*) d\mathbf{Z} + \log p(\theta^*) + \text{const} \rightarrow \max_{\theta^*}\end{aligned}$$

EM-algorithm (M-step)

$$\begin{aligned}\mathcal{L}(q, \theta) &= \int q(\mathbf{Z}) \log \frac{p(\mathbf{X}, \mathbf{Z} | \theta)}{q(\mathbf{Z})} d\mathbf{Z} \\ &= \int q(\mathbf{Z}) \log p(\mathbf{X}, \mathbf{Z} | \theta) d\mathbf{Z} + \text{const} \rightarrow \max_{\theta}\end{aligned}$$

# Mean field approximation

## Solution

$$\log q_j(\mathbf{T}_j) = \mathbb{E}_{i \neq j} \log p(\mathbf{X}, \mathbf{T}) + \text{const}$$

## EM algorithm (special case)

- ▶ Initialize  $\theta^*$ ;
- ▶ E-step

$$q(\mathbf{Z}) = \arg \max_q \mathcal{L}(q, \theta^*) = \arg \min_q KL(q||p) = p(\mathbf{Z}|\mathbf{X}, \theta^*);$$

- ▶ M-step
$$\theta^* = \arg \max_{\theta} \mathcal{L}(q, \theta);$$
- ▶ Repeat E-step and M-step until convergence.

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# IWAE

## Theorem

1.  $\log p(\mathbf{x}|\theta) \geq \mathcal{L}_K(q, \theta) \geq \mathcal{L}_M(q, \theta)$ , for  $K \geq M$ ;
2.  $\log p(\mathbf{x}|\theta) = \lim_{K \rightarrow \infty} \mathcal{L}_K(q, \theta)$  if  $\frac{p(\mathbf{x}, \mathbf{z}|\theta)}{q(\mathbf{z}|\mathbf{x})}$  is bounded.

## Proof of 1.

$$\begin{aligned}\mathcal{L}_K(q, \theta) &= \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K} \log \left( \frac{1}{K} \sum_{k=1}^K \frac{p(\mathbf{x}, \mathbf{z}_k | \theta)}{q(\mathbf{z}_k | \mathbf{x})} \right) = \\ &= \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K} \log \mathbb{E}_{k_1, \dots, k_M} \left( \frac{1}{M} \sum_{m=1}^M \frac{p(\mathbf{x}, \mathbf{z}_{k_m} | \theta)}{q(\mathbf{z}_{k_m} | \mathbf{x})} \right) \geq \\ &\geq \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K} \mathbb{E}_{k_1, \dots, k_M} \log \left( \frac{1}{M} \sum_{m=1}^M \frac{p(\mathbf{x}, \mathbf{z}_{k_m} | \theta)}{q(\mathbf{z}_{k_m} | \mathbf{x})} \right) = \\ &= \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_M} \log \left( \frac{1}{M} \sum_{m=1}^M \frac{p(\mathbf{x}, \mathbf{z}_m | \theta)}{q(\mathbf{z}_m | \mathbf{x})} \right) = \mathcal{L}_M(q, \theta)\end{aligned}$$

$$\frac{a_1 + \dots + a_K}{K} = \mathbb{E}_{k_1, \dots, k_M} \frac{a_{k_1} + \dots + a_{k_M}}{M}, \quad k_1, \dots, k_M \sim U[1, K]$$

## Theorem

1.  $\log p(\mathbf{x}|\theta) \geq \mathcal{L}_K(q, \theta) \geq \mathcal{L}_M(q, \theta)$ , for  $K \geq M$ ;
2.  $\log p(\mathbf{x}|\theta) = \lim_{K \rightarrow \infty} \mathcal{L}_K(q, \theta)$  if  $\frac{p(\mathbf{x}, \mathbf{z}|\theta)}{q(\mathbf{z}|\mathbf{x})}$  is bounded.

## Proof of 2.

Consider r.v.  $\xi_K = \frac{1}{K} \sum_{k=1}^K \frac{p(\mathbf{x}, \mathbf{z}_k|\theta)}{q(\mathbf{z}_k|\mathbf{x})}$ .

If summands are bounded, then (from the strong law of large numbers)

$$\xi_K \xrightarrow[K \rightarrow \infty]{\text{a.s.}} \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \frac{p(\mathbf{x}, \mathbf{z}|\theta)}{q(\mathbf{z}|\mathbf{x})} = p(\mathbf{x}|\theta).$$

Hence  $\mathcal{L}_K(q, \theta) = \mathbb{E} \log \xi_K$  converges to  $\log p(\mathbf{x}|\theta)$  as  $K \rightarrow \infty$ .

# Importance Weighted Autoencoders (IWAE)

## Theorem

1.  $\log p(\mathbf{x}|\theta) \geq \mathcal{L}_K(q, \theta) \geq \mathcal{L}_M(q, \theta)$ , for  $K \geq M$ ;
2.  $\log p(\mathbf{x}|\theta) = \lim_{K \rightarrow \infty} \mathcal{L}_K(q, \theta)$  if  $\frac{p(\mathbf{x}, \mathbf{z}|\theta)}{q(\mathbf{z}|\mathbf{x}, \phi)}$  is bounded.

If  $K > 1$  the bound could be tighter.

$$\mathcal{L}(q, \theta) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \log \frac{p(\mathbf{x}, \mathbf{z}|\theta)}{q(\mathbf{z}|\mathbf{x}, \phi)};$$

$$\mathcal{L}_K(q, \theta) = \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x}, \phi)} \log \left( \frac{1}{K} \sum_{k=1}^K \frac{p(\mathbf{x}, \mathbf{z}_k|\theta)}{q(\mathbf{z}_k|\mathbf{x}, \phi)} \right).$$

- ▶  $\mathcal{L}_1(q, \theta) = \mathcal{L}(q, \theta)$ ;
- ▶  $\mathcal{L}_\infty(q, \theta) = \log p(\mathbf{x}|\theta)$ .
- ▶ Which  $q^*(\mathbf{z}|\mathbf{x}, \phi)$  gives  $\mathcal{L}(q^*, \theta) = \log p(\mathbf{x}|\theta)$ ?
- ▶ Which  $q^*(\mathbf{z}|\mathbf{x}, \phi)$  gives  $\mathcal{L}(q^*, \theta) = \mathcal{L}_K(q, \theta)$ ?

# Importance Weighted Autoencoders (IWAE)

## Theorem

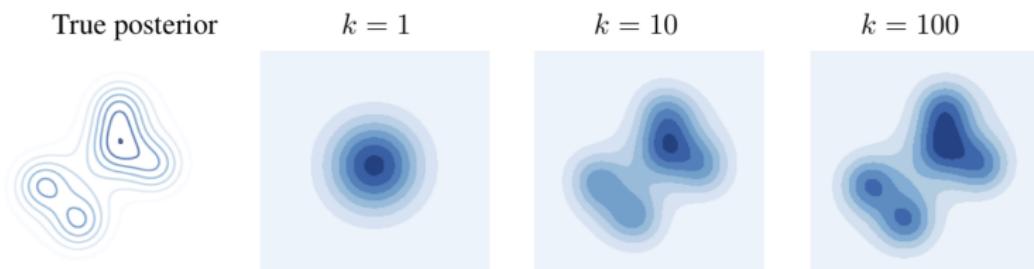
$\mathcal{L}(q^*, \theta) = \mathcal{L}_K(q, \theta)$  for the following variational distribution

$$q^*(\mathbf{z}|\mathbf{x}, \phi) = \mathbb{E}_{\mathbf{z}_2, \dots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} q_{IW}(\mathbf{z}|\mathbf{x}, \mathbf{z}_{2:K}),$$

where

$$q_{IW}(\mathbf{z}|\mathbf{x}, \mathbf{z}_{2:K}) = \frac{\frac{p(\mathbf{x}, \mathbf{z})}{q(\mathbf{z}|\mathbf{x})}}{\frac{1}{K} \sum_{k=1}^K \frac{p(\mathbf{x}, \mathbf{z}_k)}{q(\mathbf{z}_k|\mathbf{x})}} q(\mathbf{z}|\mathbf{x}) = \frac{p(\mathbf{x}, \mathbf{z})}{\frac{1}{K} \left( \frac{p(\mathbf{x}, \mathbf{z})}{q(\mathbf{z}|\mathbf{x})} + \sum_{k=2}^K \frac{p(\mathbf{x}, \mathbf{z}_k)}{q(\mathbf{z}_k|\mathbf{x})} \right)}.$$

## IWAE posterior



How to determine whether all VAE latent variables are informative?

$$A_i = \text{cov}_{\mathbf{x}} (\mathbb{E}_{q(z_i|\mathbf{x})}[z_i]) > 0.01 \Leftrightarrow z_i \text{ is active}$$

# stoch. layers	k	MNIST				OMNIGLOT			
		VAE		IWAE		VAE		IWAE	
		NLL	active units	NLL	active units	NLL	active units	NLL	active units
1	1	86.76	19	86.76	19	108.11	28	108.11	28
	5	86.47	20	85.54	22	107.62	28	106.12	34
	50	86.35	20	84.78	25	107.80	28	104.67	41
2	1	85.33	16+5	85.33	16+5	107.58	28+4	107.56	30+5
	5	85.01	17+5	83.89	21+5	106.31	30+5	104.79	38+6
	50	84.78	17+5	82.90	26+7	106.30	30+5	103.38	44+7

# Importance Weighted Autoencoders (IWAE)

## Objective

$$\mathcal{L}_K(q, \theta) = \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x}, \phi)} \log \left( \frac{1}{K} \sum_{k=1}^K \frac{p(\mathbf{x}, \mathbf{z}_k | \theta)}{q(\mathbf{z}_k | \mathbf{x}, \phi)} \right) \rightarrow \max_{\phi, \theta} .$$

## Gradient

$$\Delta_K = \nabla_{\theta, \phi} \log \left( \frac{1}{K} \sum_{k=1}^K \frac{p(\mathbf{x}, \mathbf{z}_k | \theta)}{q(\mathbf{z}_k | \mathbf{x}, \phi)} \right), \quad \mathbf{z}_k \sim q(\mathbf{z} | \mathbf{x}, \phi).$$

## Theorem

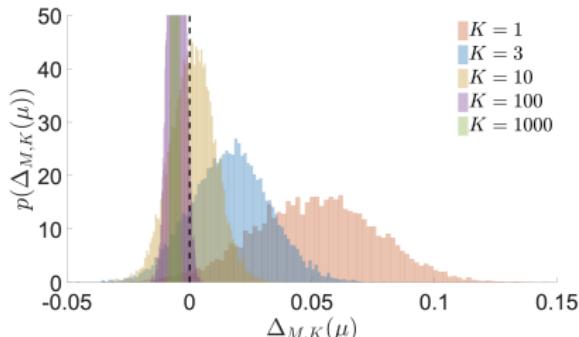
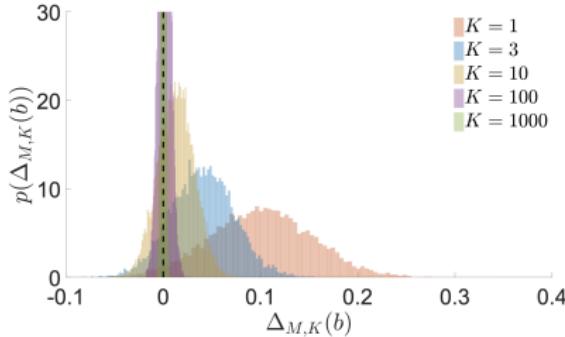
$$\text{SNR}_K = \frac{\mathbb{E}[\Delta_K]}{\sigma(\Delta_K)}; \quad \text{SNR}_K(\theta) = O(\sqrt{K}); \quad \text{SNR}_K(\phi) = O\left(\sqrt{\frac{1}{K}}\right).$$

Hence, increasing  $K$  vanishes gradient signal of inference network  $q(\mathbf{z} | \mathbf{x}, \phi)$ .

# Importance Weighted Autoencoders (IWAE)

## Theorem

$$\text{SNR}_K = \frac{\mathbb{E}[\Delta_K]}{\sigma(\Delta_K)}; \quad \text{SNR}_K(\theta) = O(\sqrt{K}); \quad \text{SNR}_K(\phi) = O\left(\sqrt{\frac{1}{K}}\right).$$

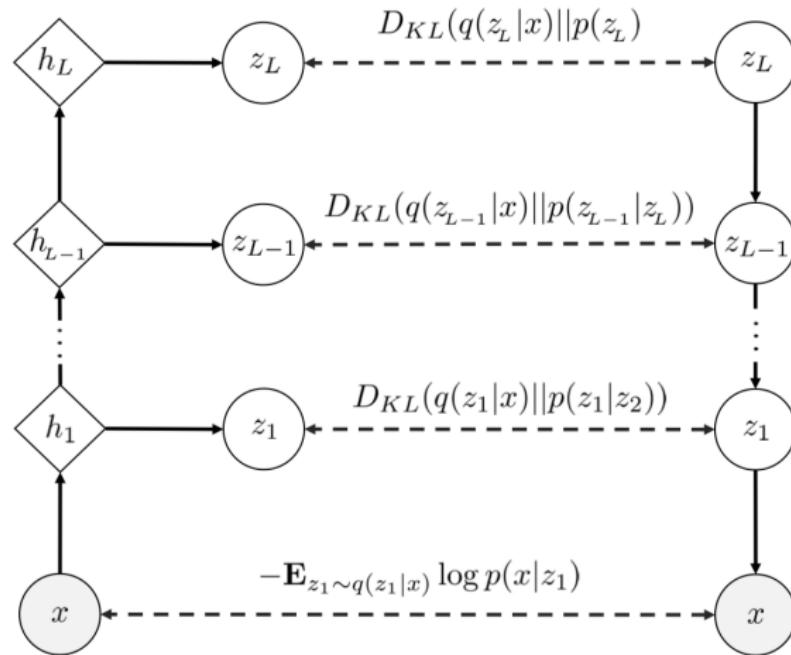


- ▶ IWAE makes the variational bound tighter and extends the class of variational distributions.
- ▶ Gradient signal becomes really small, training is complicated.
- ▶ IWAE is a standard quality measure for VAE models.

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## Hierarchical VAE



# PixelVAE, 2016

## Hierarchical decomposition

$$p(\mathbf{z}_1, \dots, \mathbf{z}_L) = p(\mathbf{z}_L)p(\mathbf{z}_{L-1}|\mathbf{z}_L)\dots p(\mathbf{z}_1, \mathbf{z}_2);$$
$$q(\mathbf{z}_1, \dots, \mathbf{z}_L|\mathbf{x}) = q(\mathbf{z}_1|\mathbf{x})\dots q(\mathbf{z}_L|\mathbf{x}).$$

## ELBO

$$\begin{aligned}\mathcal{L}(q, \theta) &= \mathbb{E}_{q(\mathbf{z}_1|\mathbf{x})} \log p(\mathbf{x}|\mathbf{z}_1, \theta) - KL(q(\mathbf{z}_1, \dots, \mathbf{z}_L|\mathbf{x})||p(\mathbf{z}_1, \dots, \mathbf{z}_L)) \\ &= \mathbb{E}_{q(\mathbf{z}_1|\mathbf{x})} \log p(\mathbf{x}|\mathbf{z}_1, \theta) - \int \prod_{j=1}^L q(\mathbf{z}_j|\mathbf{x}) \sum_{i=1}^L \log \frac{q(\mathbf{z}_i|\mathbf{x})}{p(\mathbf{z}_i|\mathbf{z}_{i+1})} d\mathbf{z}_1 \dots d\mathbf{z}_L \\ &= \mathbb{E}_{q(\mathbf{z}_1|\mathbf{x})} \log p(\mathbf{x}|\mathbf{z}_1, \theta) - \sum_{i=1}^L \int \prod_{j=1}^L q(\mathbf{z}_j|\mathbf{x}) \log \frac{q(\mathbf{z}_i|\mathbf{x})}{p(\mathbf{z}_i|\mathbf{z}_{i+1})} d\mathbf{z}_1 \dots d\mathbf{z}_L \\ &= \mathbb{E}_{q(\mathbf{z}_1|\mathbf{x})} \log p(\mathbf{x}|\mathbf{z}_1, \theta) - \sum_{i=1}^L \int q(\mathbf{z}_{i+1}|\mathbf{x}) q(\mathbf{z}_i|\mathbf{x}) \log \frac{q(\mathbf{z}_i|\mathbf{x})}{p(\mathbf{z}_i|\mathbf{z}_{i+1})} d\mathbf{z}_i d\mathbf{z}_{i+1} \\ &= \mathbb{E}_{q(\mathbf{z}_1|\mathbf{x})} \log p(\mathbf{x}|\mathbf{z}_1, \theta) - \sum_{i=1}^L \mathbb{E}_{q(\mathbf{z}_{i+1}|\mathbf{x})} [KL(q(\mathbf{z}_i|\mathbf{x})||p(\mathbf{z}_i|\mathbf{z}_{i+1}))]\end{aligned}$$

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## Posterior collapse: toy example

Let define latent variable model in the following way:

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

- ▶ prior distribution  $p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|0, \mathbf{I})$ ;
- ▶ probabilistic model  $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z}), \boldsymbol{\sigma}_{\boldsymbol{\theta}}(\mathbf{z}))$  (diagonal covariance);
- ▶ variational posterior  $q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi}) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_{\boldsymbol{\phi}}(\mathbf{x}), \boldsymbol{\sigma}_{\boldsymbol{\phi}}(\mathbf{x}))$  (diagonal covariance).

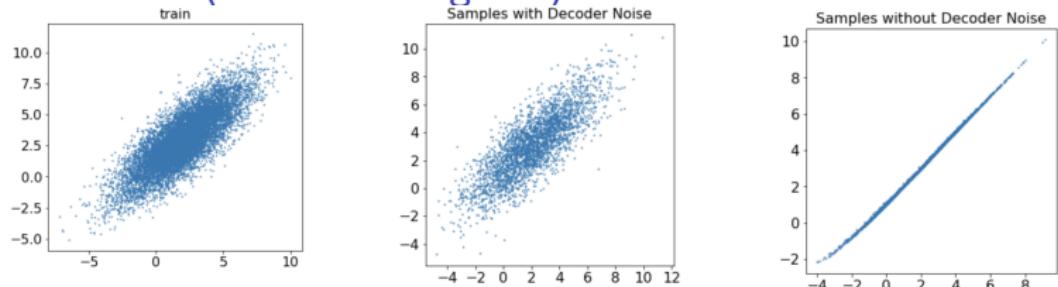
Let data distribution is  $\pi(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$ . Possible cases:

- ▶ covariance matrix  $\boldsymbol{\Sigma}$  is diagonal (univariate case);
- ▶ covariance matrix  $\boldsymbol{\Sigma}$  is **not** diagonal (multivariate case).

What is the difference?

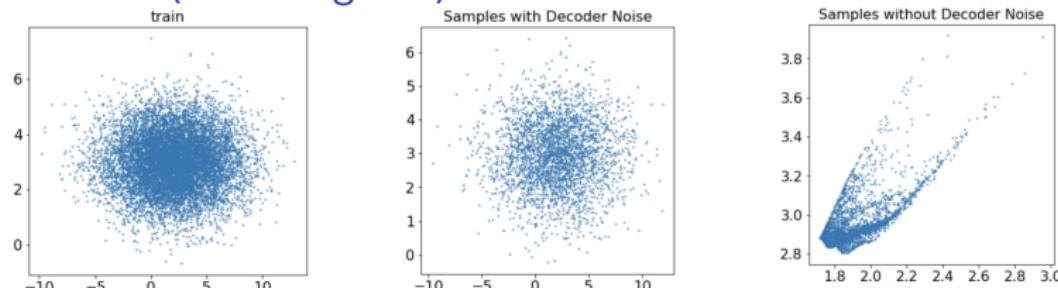
# Posterior collapse: toy example + VLAE

## Multivariate ( $\Sigma$ is non-diagonal)



The encoder uses latent variables to model data.

## Univariate ( $\Sigma$ is diagonal)



Latent variables are not used, since the decoder could model the data without the encoder.

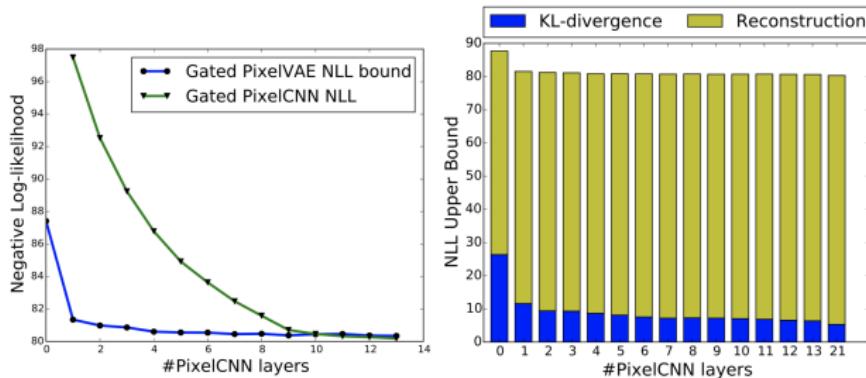
# PixelVAE

## Autoregressive decoder

$$p(\mathbf{x}|\mathbf{z}, \theta) = \prod_{j=1}^m p(x_j|\mathbf{x}_{1:j-1}, \mathbf{z}, \theta)$$

- ▶ Global structure is captured by latent variables.
- ▶ Local statistics are captured by limited receptive field autoregressive model.

## MNIST results



# Variational Lossy AutoEncoder

Lossy code via explicit information placement

$$p(\mathbf{x}|\mathbf{z}, \theta) = \prod_{i=1}^m p(x_i|\mathbf{z}, \mathbf{x}_{\text{WindowAround}(i)}, \theta).$$

- ▶  $\text{WindowAround}(i)$  restricts the receptive field (it forbids to represent arbitrarily complex distribution over  $\mathbf{x}$  without dependence on  $\mathbf{z}$ ).
- ▶ Local statistics of 2D images (texture) will be modeled by a small local window.
- ▶ Global structural information (shapes) is long-range dependency that can only be communicated through latent code  $\mathbf{z}$ .

# Variational Lossy AutoEncoder

- ▶ Can VLAE learn lossy codes that encode global statistics?
- ▶ Does using AF priors improves upon using IAF posteriors as predicted by theory?
- ▶ Does using autoregressive decoding distributions improve density estimation performance?

## CIFAR10

### MNIST

Model	NLL Test
Normalizing flows (Rezende & Mohamed, 2015)	85.10
DRAW (Gregor et al., 2015)	< 80.97
Discrete VAE (Rollef, 2016)	81.01
PixelRNN (van den Oord et al., 2016a)	79.20
IAF VAE (Kingma et al., 2016)	79.88
AF VAE	79.30
VLAE	<b>79.03</b>

Method	bits/dim $\leq$
<i>Results with tractable likelihood models:</i>	
Uniform distribution [1]	8.00
Multivariate Gaussian [1]	4.70
NICE [2]	4.48
Deep GMMS [3]	4.00
Real NVP [4]	3.49
PixelCNN [1]	3.14
Gated PixelCNN [5]	3.03
PixelRNN [1]	3.00
PixelCNN++ [6]	<b>2.92</b>
<i>Results with variationally trained latent-variable models:</i>	
Deep Diffusion [7]	5.40
Convolutional DRAW [8]	3.58
ResNet VAE with IAF [9]	3.11
ResNet VLAE	3.04
DenseNet VLAE	<b>2.95</b>

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## Flows intuition

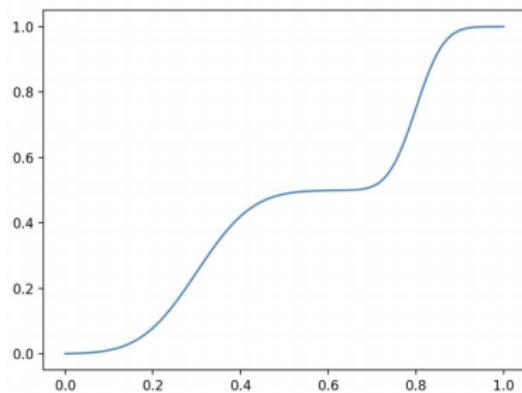
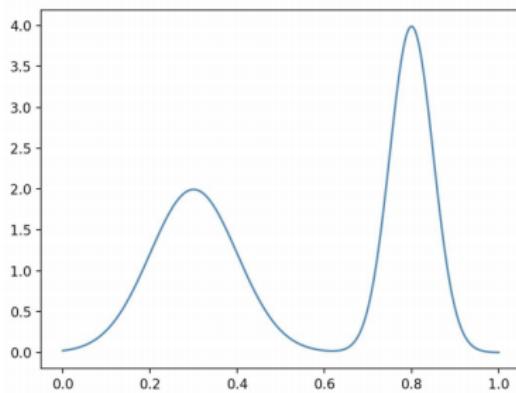
Let  $\xi$  be a random variable with density  $p(\xi)$ . Then

$$\eta = F(\xi) = \int_{-\infty}^{\xi} p(t)dt \sim U[0, 1].$$

$$P(\eta < y) = P(F(\xi) < y) = P(\xi < F^{-1}(y)) = F(F^{-1}(y)) = y$$

Hence

$$\eta \sim U[0, 1]; \quad \xi = F^{-1}(\eta) \quad \Rightarrow \quad \xi \sim p(\xi).$$



## Flows intuition

- ▶ Let  $z \sim p(z)$  is a random variable with base distribution  $p(z) = U[0, 1]$ .
- ▶ Let  $x \sim p(x)$  is a random variable with complex distribution  $p(x)$  and cdf  $F(x)$ .
- ▶ Then noise variable  $z$  can be transformed to  $x$  using inverse cdf  $F^{-1}$  ( $x = F^{-1}(z)$ ).

How to transform random variable  $z$  which has a distribution different from uniform to  $x$ ?

- ▶ Let  $z \sim p(z)$  is a random variable with base distribution  $p(z)$  and cdf  $G(z)$ .
- ▶ Then  $z_0 = G(z)$  has base distribution  $p(z_0) = U[0, 1]$ .
- ▶ Let  $x \sim p(x)$  is a random variable with complex distribution  $p(x)$  and cdf  $F(x)$ .
- ▶ Then noise variable  $z$  can be transformed to  $x$  using cdf  $G$  and inverse cdf  $F^{-1}$  ( $x = F^{-1}(z_0) = F^{-1}(G(z))$ ).

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# Residual Flows

## Matrix determinant lemma

$$\det(\mathbf{I}_m + \mathbf{V}\mathbf{W}^T) = \det(\mathbf{I}_d + \mathbf{W}^T\mathbf{V}), \quad \text{where } \mathbf{V}, \mathbf{W} \in \mathbb{R}^{m \times d}.$$

## Planar flow

$$\mathbf{x} = g(\mathbf{z}, \boldsymbol{\theta}) = \mathbf{z} + \mathbf{v} \sigma(\mathbf{w}^T \mathbf{z} + b).$$

Here  $\boldsymbol{\theta} = \{\mathbf{v}, \mathbf{w}, b\}$ ,  $\sigma(\cdot)$  is a smooth element-wise non-linearity.

$$\left| \det \left( \frac{\partial g(\mathbf{z}, \boldsymbol{\theta})}{\partial \mathbf{z}} \right) \right| = \left| \det (\mathbf{I} + \sigma'(\mathbf{w}^T \mathbf{z} + b) \mathbf{v} \mathbf{w}^T) \right| = \left| 1 + \sigma'(\mathbf{w}^T \mathbf{z} + b) \mathbf{w}^T \mathbf{v} \right|$$

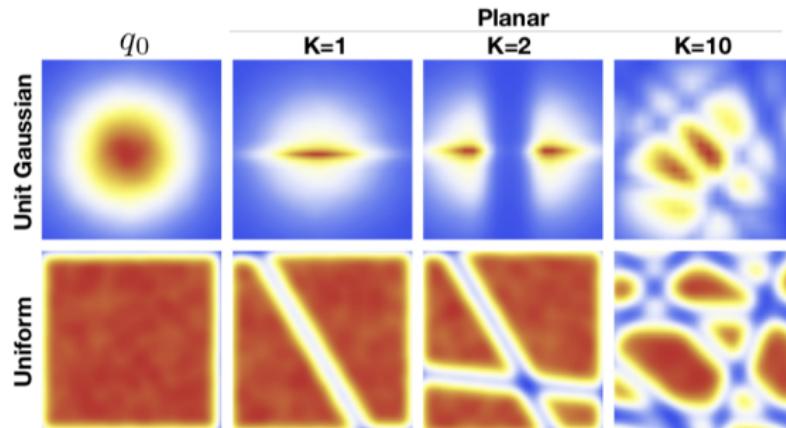
The transformation is invertible, for example, if

$$\sigma = \tanh; \quad \sigma'(\mathbf{w}^T \mathbf{z} + b) \mathbf{w}^T \mathbf{v} \geq -1.$$

# Residual Flows

## Expressiveness of planar flows

$$\mathbf{z}_K = g_1 \circ \cdots \circ g_K(\mathbf{z}); \quad g_k = g(\mathbf{z}_k, \theta_k) = \mathbf{z}_k + \mathbf{v}_k \sigma(\mathbf{w}_k^T \mathbf{z}_k + b_k).$$



Sylvester flow: planar flow extension

$$g(\mathbf{z}, \theta) = \mathbf{z} + \mathbf{V} \sigma(\mathbf{W}^T \mathbf{z} + \mathbf{b}).$$

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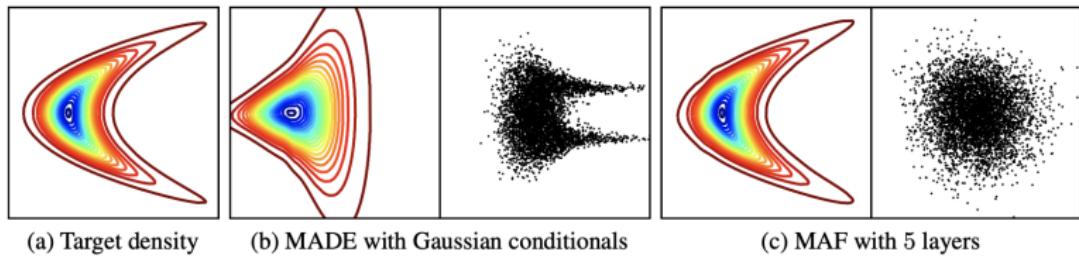
Rezende D. J., Mohamed S. Variational Inference with Normalizing Flows, 2015  
Berg R. et al. Sylvester normalizing flows for variational inference, 2018

# Masked autoregressive flow (MAF)

## Gaussian autoregressive model

$$p(\mathbf{x}|\theta) = \prod_{j=1}^m p(x_j|\mathbf{x}_{1:j-1}, \theta) = \prod_{j=1}^m \mathcal{N}(x_j | \mu_j(\mathbf{x}_{1:j-1}), \sigma_j^2(\mathbf{x}_{1:j-1})).$$

We could use MADE for the conditionals. Samples from the base distribution could be an indicator of how good the flow was fitted.



MAF is just a stacked MADE model with different ordering.

- ▶ Parallel density estimation.
- ▶ Sequential sampling.

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## Autoregressive flows

$$x_j = \tau(z_j, c(\mathbf{z}_{1:j-1})) \Leftrightarrow z_j = \tau^{-1}(x_j, c(\mathbf{z}_{1:j-1}))$$

- ▶  $\tau(\cdot, \cdot)$  – coupling law (invertible by first argument, differentiable).
- ▶  $c(\cdot)$  – coupling function (do not need to be invertible, could be neural network).

### Coupling law $\tau(\cdot, \cdot)$

- ▶  $\tau(x, c) = x + c$  – additive;
- ▶  $\tau(x, c) = x \odot c_1 + c_2$  – affine.

What is the Jacobian for the additive/affine coupling law?

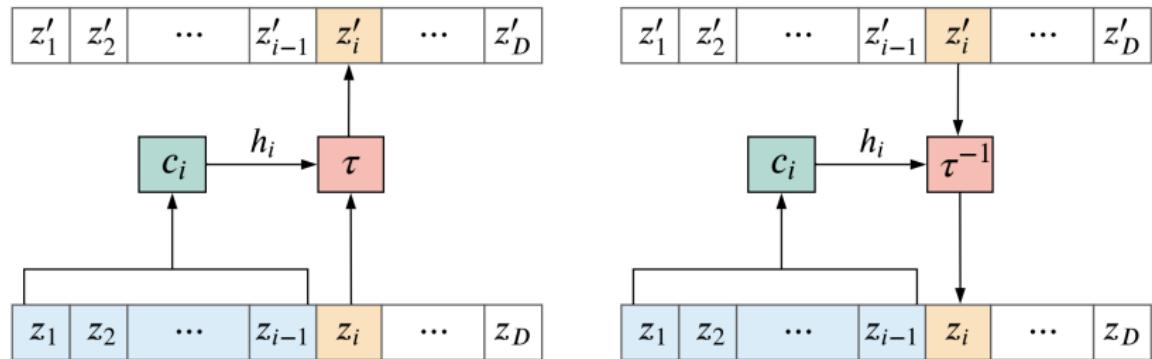
### Jacobian

$$\det \left( \frac{\partial \mathbf{x}}{\partial \mathbf{z}} \right) = \prod_{j=1}^m \frac{\partial x_j}{\partial z_j} = \prod_{j=1}^m \frac{\partial \tau(z_j, c(\mathbf{z}_{1:j-1}))}{\partial z_j}$$

# Autoregressive flows

## Forward and inverse transforms

$$x_j = \tau(z_j, c(\mathbf{z}_{1:j-1})) \Leftrightarrow z_j = \tau^{-1}(x_j, c(\mathbf{z}_{1:j-1}))$$



- ▶ Forward transform is **not sequential**.
- ▶ Inverse transform is **sequential**.

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# MAF/IAF pros and cons

## MAF

- ▶ Sampling is slow.
- ▶ Likelihood evaluation is fast.

## IAF

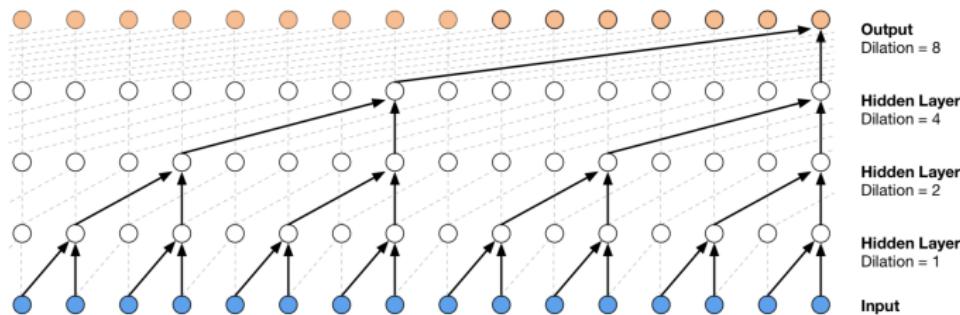
- ▶ Sampling is fast.
- ▶ Likelihood evaluation is slow.

How to take the best of both worlds?

## WaveNet

Autoregressive model with caused dilated convolutions for raw audio waveforms generation.

$$p(\mathbf{x}|\theta) = \prod_{t=1}^T p(x_t|\mathbf{x}_{1:t-1}, \theta).$$



# AF vs IAF vs RealINVP

## MADE/AF

$$\mathbf{x} = \sigma(\mathbf{z}) \odot \mathbf{z} + \mu(\mathbf{x}).$$

Estimating the density  $p(\mathbf{x}|\theta)$  - 1 pass, sampling -  $m$  passes.

## IAF

$$\mathbf{x} = \tilde{\sigma}(\mathbf{z}) \odot \mathbf{z} + \tilde{\mu}(\mathbf{z}).$$

Estimating the density  $p(\mathbf{x}|\theta)$  -  $m$  passes, sampling - 1 pass.

## RealINVP

$$\begin{cases} \mathbf{x}_{1:d} &= \mathbf{z}_{1:d}; \\ \mathbf{x}_{d:m} &= \mathbf{z}_{d:m} \odot c_1(\mathbf{z}_{1:d}, \theta) + c_2(\mathbf{z}_{1:d}, \theta). \end{cases}$$

# AF vs IAF vs RealINVP

## RealINVP

$$\begin{cases} \mathbf{x}_{1:d} = \mathbf{z}_{1:d}; \\ \mathbf{x}_{d:m} = \mathbf{z}_{d:m} \odot c_1(\mathbf{z}_{1:d}, \boldsymbol{\theta}) + c_2(\mathbf{z}_{1:d}, \boldsymbol{\theta}). \end{cases}$$

- ▶ Calculating the density  $p(\mathbf{x}|\boldsymbol{\theta})$  - 1 pass.
- ▶ Sampling - 1 pass.

RealINVP is a special case of AF and IAF:

## AF

$$\begin{cases} \mu_j = 0, \sigma_j = 1, j = 1, \dots, d; \\ \mu_j, \sigma_j - \text{functions of } \mathbf{x}_{1:d}, j = d + 1, \dots, m. \end{cases}$$

## IAF

$$\begin{cases} \tilde{\mu}_j = 0, \tilde{\sigma}_j = 1, j = 1, \dots, d; \\ \tilde{\mu}_j, \tilde{\sigma}_j - \text{functions of } \mathbf{z}_{1:d}, j = d + 1, \dots, m. \end{cases}$$

# Linear flows

## RealNVP

$$\begin{cases} \mathbf{z}_{1:d} = \mathbf{x}_{1:d}; \\ \mathbf{z}_{d:m} = \tau(\mathbf{x}_{d:m}, c(\mathbf{x}_{1:d})); \end{cases} \Leftrightarrow \begin{cases} \mathbf{x}_{1:d} = \mathbf{z}_{1:d}; \\ \mathbf{x}_{d:m} = \tau^{-1}(\mathbf{z}_{d:m}, c(\mathbf{z}_{1:d})). \end{cases}$$

- ▶ First step is a **split** operator which decouples a variable into 2 subparts:  $\mathbf{x}_1$  and  $\mathbf{x}_2$  (usually channel-wise).
- ▶ We should **permute** components between different layers.

$$\mathbf{z} = \mathbf{W}\mathbf{x}, \quad \mathbf{W} \in \mathbb{R}^{m \times m}$$

In general, we need  $O(m^3)$  to invert matrix.

## Invertibility

- ▶ Diagonal matrix  $O(m)$ .
- ▶ Triangular matrix  $O(m^2)$ .
- ▶ It is impossible to parametrize all invertible matrices.

## Parallel WaveNet

- ▶ 24kHz instead of 16kHz using increased dilated convolution filter size from 2 to 3.
- ▶ 16-bit signals with mixture of logistics instead of 8-bit signal with 256-way categorical distribution.

### Probability density distillation

1. Train usual WaveNet (MAF) via MLE (teacher network).
2. Train IAF WaveNet (student network), which attempts to match the probability of its own samples under the distribution learned by the teacher.

### Student objective

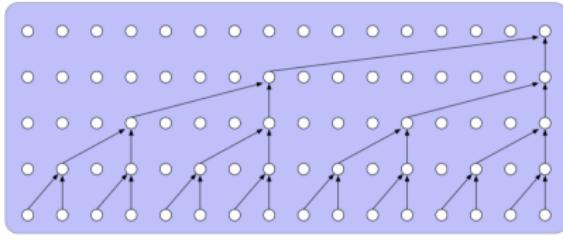
$$KL(p_s || p_t) = H(p_s, p_t) - H(p_s).$$

More than 1000x speed-up relative to original WaveNet!

# Parallel WaveNet

## WaveNet Teacher

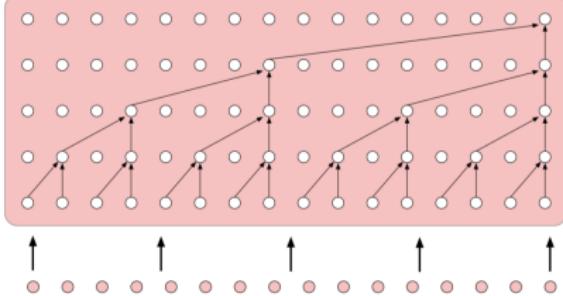
Linguistic features  $\dashrightarrow$



Teacher Output  
 $P(x_i | x_{<i})$

## WaveNet Student

Linguistic features  $\dashrightarrow$



Generated Samples  
 $x_i = g(z_i | z_{<i})$

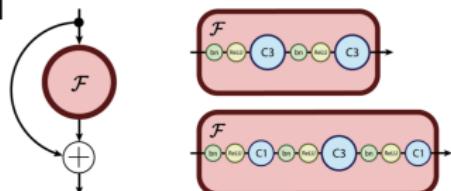
Student Output  
 $P(x_i | z_{<i})$

Input noise  
 $z_i$

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- ▶ Modern neural networks are trained via backpropagation.
- ▶ Residual networks are state of the art in image classification.
- ▶ Backpropagation requires storing the network activations.



## Problem

Storing the activations imposes an increasing memory burden.

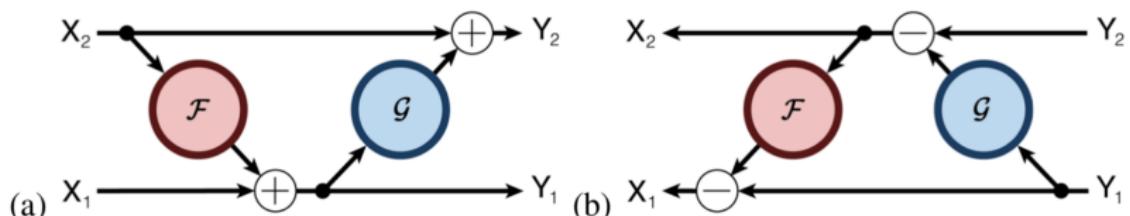
GPUs have limited memory capacity, leading to constraints often exceeded by state-of-the-art architectures (with thousand layers).

## NICE

$$\begin{cases} \mathbf{z}_1 = \mathbf{x}_1; \\ \mathbf{z}_2 = \mathbf{x}_2 + \mathcal{F}(\mathbf{x}_1, \theta); \end{cases} \Leftrightarrow \begin{cases} \mathbf{x}_1 = \mathbf{z}_1; \\ \mathbf{x}_2 = \mathbf{z}_2 - \mathcal{F}(\mathbf{z}_1, \theta). \end{cases}$$

## RevNet

$$\begin{cases} \mathbf{y}_1 = \mathbf{x}_1 + \mathcal{F}(\mathbf{x}_2, \theta); \\ \mathbf{y}_2 = \mathbf{x}_2 + \mathcal{G}(\mathbf{y}_1, \theta); \end{cases} \Leftrightarrow \begin{cases} \mathbf{x}_2 = \mathbf{y}_2 - \mathcal{F}(\mathbf{y}_1, \theta); \\ \mathbf{x}_1 = \mathbf{y}_1 - \mathcal{G}(\mathbf{x}_2, \theta). \end{cases}$$



Architecture	CIFAR-10 [15]		CIFAR-100 [15]	
	ResNet	RevNet	ResNet	RevNet
32 (38)	<b>7.14%</b>	7.24%	29.95%	<b>28.96%</b>
110	<b>5.74%</b>	5.76%	26.44%	<b>25.40%</b>
164	5.24%	<b>5.17%</b>	<b>23.37%</b>	23.69%

- ▶ If the network contains non-reversible blocks (poolings, strides), activations for these blocks should be stored.
- ▶ To avoid storing activations in the modern frameworks, the backward pass should be manually redefined.

## Hypothesis

The success of deep convolutional networks is based on progressively discarding uninformative variability about the input with respect to the problem at hand.

- ▶ It is difficult to recover images from their hidden representations.
- ▶ Information bottleneck principle: an optimal representation must reduce the MI between an input and its representation to reduce uninformative variability + maximize the MI between the output and its representation to preserve each class from collapsing onto other classes.

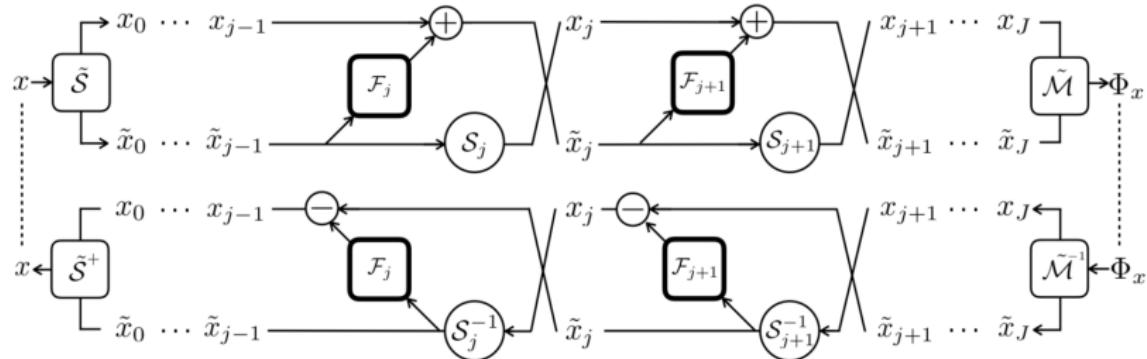
## Hypothesis

The success of deep convolutional networks is based on progressively discarding uninformative variability about the input with respect to the problem at hand.

## Idea

Build a cascade of homeomorphic layers (i-RevNet), a network that can be fully inverted up to the final projection onto the classes, i.e. no information is discarded.

# i-RevNet, 2018



Architecture	Injective	Bijective	Top-1 error	Parameters
ResNet	-	-	24.7	26M
RevNet	-	-	25.2	28M
<i>i</i> -RevNet (a)	yes	-	24.7	181M
<i>i</i> -RevNet (b)	yes	yes	26.7	29M

## Flow-based variational dequantization

$$\log P(\mathbf{x}|\theta) \geq \int p(\epsilon) \log \left( \frac{p(\mathbf{x} + g(\epsilon, \mathbf{x}, \lambda))}{p(\epsilon) \cdot |\det \mathbf{J}_g|^{-1}} \right) d\epsilon.$$

Table 1. Unconditional image modeling results in bits/dim

Model family	Model	CIFAR10	ImageNet 32x32	ImageNet 64x64
Non-autoregressive	RealNVP (Dinh et al., 2016)	3.49	4.28	—
	Glow (Kingma & Dhariwal, 2018)	3.35	4.09	3.81
	IAF-VAE (Kingma et al., 2016)	3.11	—	—
	<b>Flow++ (ours)</b>	<b>3.08</b>	<b>3.86</b>	<b>3.69</b>
Autoregressive	Multiscale PixelCNN (Reed et al., 2017)	—	3.95	3.70
	PixelCNN (van den Oord et al., 2016b)	3.14	—	—
	PixelRNN (van den Oord et al., 2016b)	3.00	3.86	3.63
	Gated PixelCNN (van den Oord et al., 2016c)	3.03	3.83	3.57
	PixelCNN++ (Salimans et al., 2017)	2.92	—	—
	Image Transformer (Parmar et al., 2018)	2.90	3.77	—
	PixelSNAIL (Chen et al., 2017)	2.85	3.80	3.52

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## ELBO interpretations

$$\log p(\mathbf{x}|\theta) = \mathcal{L}(q, \theta) + KL(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}|\mathbf{x}, \theta)).$$

$$\mathcal{L}(q, \theta) = \int q(\mathbf{z}|\mathbf{x}, \phi) \log \frac{p(\mathbf{x}, \mathbf{z}|\theta)}{q(\mathbf{z}|\mathbf{x}, \phi)} d\mathbf{z}.$$

- ▶ Evidence minus posterior KL

$$\mathcal{L}(q, \theta) = \log p(\mathbf{x}|\theta) - KL(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}|\mathbf{x}, \theta)).$$

- ▶ Average negative energy plus entropy

$$\begin{aligned}\mathcal{L}(q, \theta) &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} [\log p(\mathbf{x}, \mathbf{z}|\theta) - \log q(\mathbf{z}|\mathbf{x}, \phi)] \\ &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \log p(\mathbf{x}, \mathbf{z}|\theta) + \mathbb{H}[q(\mathbf{z}|\mathbf{x}, \phi)].\end{aligned}$$

- ▶ Average reconstruction minus KL to prior

$$\begin{aligned}\mathcal{L}(q, \theta) &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} [\log p(\mathbf{x}|\mathbf{z}, \theta) + \log p(\mathbf{z}) - \log q(\mathbf{z}|\mathbf{x}, \phi)] \\ &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \log p(\mathbf{x}|\mathbf{z}, \theta) - KL(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z})).\end{aligned}$$

# ELBO surgery, 2016

$$\mathcal{L}(q, \theta) = \int q(\mathbf{Z}|\mathbf{X}) \log \frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z}|\mathbf{X})} d\mathbf{Z}.$$

## ELBO interpretations

- ▶ Evidence minus posterior KL

$$\mathcal{L}(q, \theta) = \log p(\mathbf{X}|\theta) - KL(q(\mathbf{Z}|\mathbf{X})||p(\mathbf{Z}|\mathbf{X}, \theta)).$$

- ▶ Average negative energy plus entropy

$$\mathcal{L}(q, \theta) = \mathbb{E}_{q(\mathbf{Z}|\mathbf{X})} p(\mathbf{X}, \mathbf{Z}|\theta) + \mathbb{H}[q(\mathbf{Z}|\mathbf{X})].$$

- ▶ Average term-by-term reconstruction minus KL to prior

$$\mathcal{L}(q, \theta) = \frac{1}{n} \sum_{i=1}^n [\mathbb{E}_{q(\mathbf{z}_i|\mathbf{x}_i)} \log p(\mathbf{x}_i|\mathbf{z}_i, \theta) - KL(q(\mathbf{z}_i|\mathbf{x}_i)||p(\mathbf{z}_i))].$$

# ELBO surgery, 2016

$$\mathcal{L}(q, \theta) = \frac{1}{n} \sum_{i=1}^n [\mathbb{E}_{q(\mathbf{z}_i|\mathbf{x}_i)} \log p(\mathbf{x}_i|\mathbf{z}_i, \theta) - KL(q(\mathbf{z}_i|\mathbf{x}_i)||p(\mathbf{z}_i))].$$

## Theorem

$$\frac{1}{n} \sum_{i=1}^n KL(q(\mathbf{z}_i|\mathbf{x}_i)||p(\mathbf{z}_i)) = KL(q(\mathbf{z})||p(\mathbf{z})) + \mathbb{I}_{q(i,\mathbf{z})}[i, \mathbf{z}],$$

where  $i$  is treated as random variable:

$$q(i, \mathbf{z}) = q(i)q(\mathbf{z}|i); \quad p(i, \mathbf{z}) = p(i)p(\mathbf{z}); \quad q(i) = p(i) = \frac{1}{n}; \quad q(\mathbf{z}|i) = q(\mathbf{z}|\mathbf{x}_i).$$

$$q(\mathbf{z}) = \sum_{i=1}^n q(i, \mathbf{z}) = \frac{1}{n} \sum_{i=1}^n q(\mathbf{z}|\mathbf{x}_i); \quad \mathbb{I}_{q(i,\mathbf{z})}[i, \mathbf{z}] = \mathbb{E}_{q(i,\mathbf{z})} \log \frac{q(i, \mathbf{z})}{q(i)q(\mathbf{z})}.$$

# ELBO surgery, 2016

## Theorem

$$\frac{1}{n} \sum_{i=1}^n KL(q(\mathbf{z}_i | \mathbf{x}_i) || p(\mathbf{z}_i)) = KL(q(\mathbf{z}) || p(\mathbf{z})) + \mathbb{I}_{q(i, \mathbf{z})}[i, \mathbf{z}].$$

## Proof

$$\begin{aligned}\frac{1}{n} \sum_{i=1}^n KL(q(\mathbf{z}_i | \mathbf{x}_i) || p(\mathbf{z}_i)) &= \sum_{i=1}^n \int q(i) q(\mathbf{z}|i) \log \frac{q(\mathbf{z}|i)}{p(\mathbf{z})} d\mathbf{z} = \\&= \sum_{i=1}^n \int q(i, \mathbf{z}) \log \frac{q(i, \mathbf{z})}{p(\mathbf{z})p(i)} d\mathbf{z} = \int \sum_{i=1}^n q(i, \mathbf{z}) \log \frac{q(\mathbf{z})q(i|\mathbf{z})}{p(\mathbf{z})p(i)} d\mathbf{z} = \\&= \int q(\mathbf{z}) \log \frac{q(\mathbf{z})}{p(\mathbf{z})} d\mathbf{z} + \int \sum_{i=1}^n q(i|\mathbf{z})q(\mathbf{z}) \log \frac{q(i|\mathbf{z})}{p(i)} d\mathbf{z} = \\&= KL(q(\mathbf{z}) || p(\mathbf{z})) - \mathbb{E}_{q(\mathbf{z})} \mathbb{H}[q(i|\mathbf{z})] + \log n.\end{aligned}$$

# ELBO surgery, 2016

## Theorem

$$\frac{1}{n} \sum_{i=1}^n KL(q(\mathbf{z}_i | \mathbf{x}_i) || p(\mathbf{z}_i)) = KL(q(\mathbf{z}) || p(\mathbf{z})) + \mathbb{I}_{q(i, \mathbf{z})}[i, \mathbf{z}].$$

## Proof (continued)

$$\frac{1}{n} \sum_{i=1}^n KL(q(\mathbf{z}_i | \mathbf{x}_i) || p(\mathbf{z}_i)) = KL(q(\mathbf{z}) || p(\mathbf{z})) - \mathbb{E}_{q(\mathbf{z})} \mathbb{H}[q(i|\mathbf{z})] + \log n$$

$$\begin{aligned}\mathbb{I}_{q(i, \mathbf{z})}[i, \mathbf{z}] &= \mathbb{E}_{q(i, \mathbf{z})} \log \frac{q(i, \mathbf{z})}{q(i)q(\mathbf{z})} = \mathbb{E}_{q(\mathbf{z})} \mathbb{E}_{q(i|\mathbf{z})} \log \frac{q(i|\mathbf{z})q(\mathbf{z})}{q(i)q(\mathbf{z})} = \\ &= \mathbb{E}_{q(\mathbf{z})} \mathbb{E}_{q(i|\mathbf{z})} \log \frac{q(i|\mathbf{z})}{q(i)} = -\mathbb{E}_{q(\mathbf{z})} \mathbb{H}[q(i|\mathbf{z})] + \log n.\end{aligned}$$

## Learnable VAE prior

### Optimal prior

$$KL(q_{\text{agg}}(\mathbf{z}) || p(\mathbf{z})) = 0 \Leftrightarrow p(\mathbf{z}) = q_{\text{agg}}(\mathbf{z}) = \frac{1}{n} \sum_{i=1}^n q(\mathbf{z} | \mathbf{x}_i).$$

### Mixture of Gaussians

$$p(\mathbf{z} | \boldsymbol{\lambda}) = \sum_{k=1}^K w_k \mathcal{N}(\mathbf{z} | \boldsymbol{\mu}_k, \boldsymbol{\sigma}_k^2), \quad \boldsymbol{\lambda} = \{w_k, \boldsymbol{\mu}_k, \boldsymbol{\sigma}_k\}_{k=1}^K.$$

### Variational Mixture of posteriors (VampPrior)

$$p(\mathbf{z} | \boldsymbol{\lambda}) = \frac{1}{K} \sum_{k=1}^K q(\mathbf{z} | \mathbf{u}_k),$$

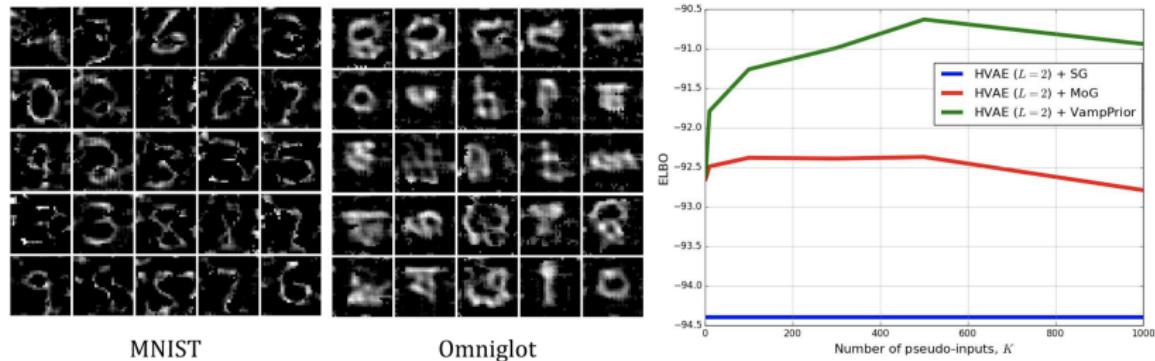
where  $\boldsymbol{\lambda} = \{\mathbf{u}_1, \dots, \mathbf{u}_K\}$  are trainable pseudo-inputs.

- ▶ Multimodal  $\Rightarrow$  prevents over-regularization;.
- ▶  $K \ll n \Rightarrow$  prevents from potential overfitting + less expensive to train.

# VampPrior

- ▶ Do we really need the multimodal prior?
- ▶ Is it beneficial to couple the prior with the variational posterior or the MoG prior is enough?

## Results



**Top row:** generated images by PixelHVAE + VampPrior for chosen pseudo-input in the left top corner.

**Bottom row:** pseudo-inputs for different datasets.

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# InfoGAN

## GAN objective

$$\min_G \max_D V(G, D)$$

$$V(G, D) = \mathbb{E}_{\pi(x)} \log D(x) + \mathbb{E}_{p(z)} \log(1 - D(G(z)))$$

Latent vector  $\mathbf{z}$  is not imposed to be disentangled.

InfoGAN decomposes input vector:

- ▶  $\mathbf{z}$  – incompressible noise;
- ▶  $\mathbf{c}$  – structured latent code  $p(\mathbf{c}) = \prod_{j=1}^d p(c_j)$ .

## Information-theoretic regularization

$$\max I(\mathbf{c}, G(\mathbf{z}, \mathbf{c}))$$

Information in the latent code  $\mathbf{c}$  should not be lost in the  
generation process.

Chen X. et al. InfoGAN: Interpretable Representation Learning by Information Maximizing Generative Adversarial Nets, 2016

# InfoGAN

## Objective

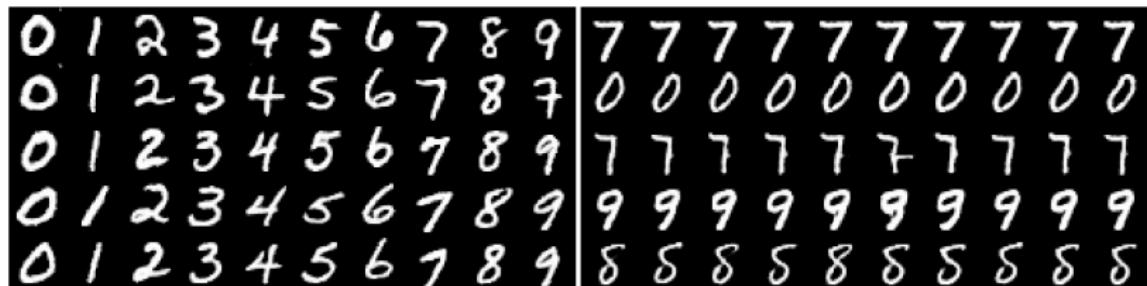
$$\min_G \max_D V(G, D) - \lambda I(\mathbf{c}, G(\mathbf{z}, \mathbf{c}))$$

## Variational Information Maximization

$$\begin{aligned} I(\mathbf{c}, G(\mathbf{z}, \mathbf{c})) &= H(\mathbf{c}) - H(\mathbf{c}|G(\mathbf{z}, \mathbf{c})) = \\ &= H(\mathbf{c}) + \mathbb{E}_{\mathbf{x} \sim G(\mathbf{z}, \mathbf{c})} [\mathbb{E}_{\mathbf{c}' \sim p(\mathbf{c}|\mathbf{x})} \log p(\mathbf{c}'|\mathbf{x})] = \\ &= H(\mathbf{c}) + \mathbb{E}_{\mathbf{x} \sim G(\mathbf{z}, \mathbf{c})} KL(p(\mathbf{c}'|\mathbf{x}) || q(\mathbf{z}'|\mathbf{x})) + \\ &\quad + \mathbb{E}_{\mathbf{x} \sim G(\mathbf{z}, \mathbf{c})} \mathbb{E}_{\mathbf{c}' \sim p(\mathbf{c}|\mathbf{x})} \log q(\mathbf{c}'|\mathbf{x}) \geq \\ &\geq H(\mathbf{c}) + \mathbb{E}_{\mathbf{x} \sim G(\mathbf{z}, \mathbf{c})} \mathbb{E}_{\mathbf{c}' \sim p(\mathbf{c}|\mathbf{x})} \log q(\mathbf{c}'|\mathbf{x}) = \\ &\quad H(\mathbf{c}) + \mathbb{E}_{\mathbf{c} \sim p(\mathbf{c})} \mathbb{E}_{\mathbf{x} \sim G(\mathbf{z}, \mathbf{c})} \log q(\mathbf{c}|\mathbf{x}) \end{aligned}$$

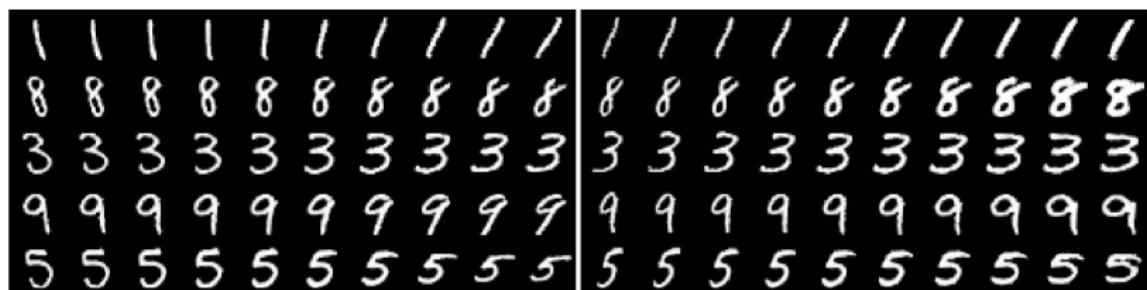
# InfoGAN

## Latent codes on MNIST



(a) Varying  $c_1$  on InfoGAN (Digit type)

(b) Varying  $c_1$  on regular GAN (No clear meaning)



(c) Varying  $c_2$  from  $-2$  to  $2$  on InfoGAN (Rotation)

(d) Varying  $c_3$  from  $-2$  to  $2$  on InfoGAN (Width)

# InfoGAN

## Latent codes on 3D Faces



(a) Azimuth (pose)

(b) Elevation



(c) Lighting

(d) Wide or Narrow

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Chen X. et al. InfoGAN: Interpretable Representation Learning by Information Maximizing Generative Adversarial Nets, 2016

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# Disentangled representations

**Representation learning** is looking for an interpretable representation of the independent data generative factors.

## Disentanglement informal definition

Every single latent unit are sensitive to changes in a single generative factor, while being invariant to changes in other factors.

## ELBO objective

$$\mathcal{L}(q, \theta, \beta) = \mathbb{E}_{q(z|x)} \log p(x|z, \theta) - \beta \cdot KL(q(z|x)||p(z)).$$

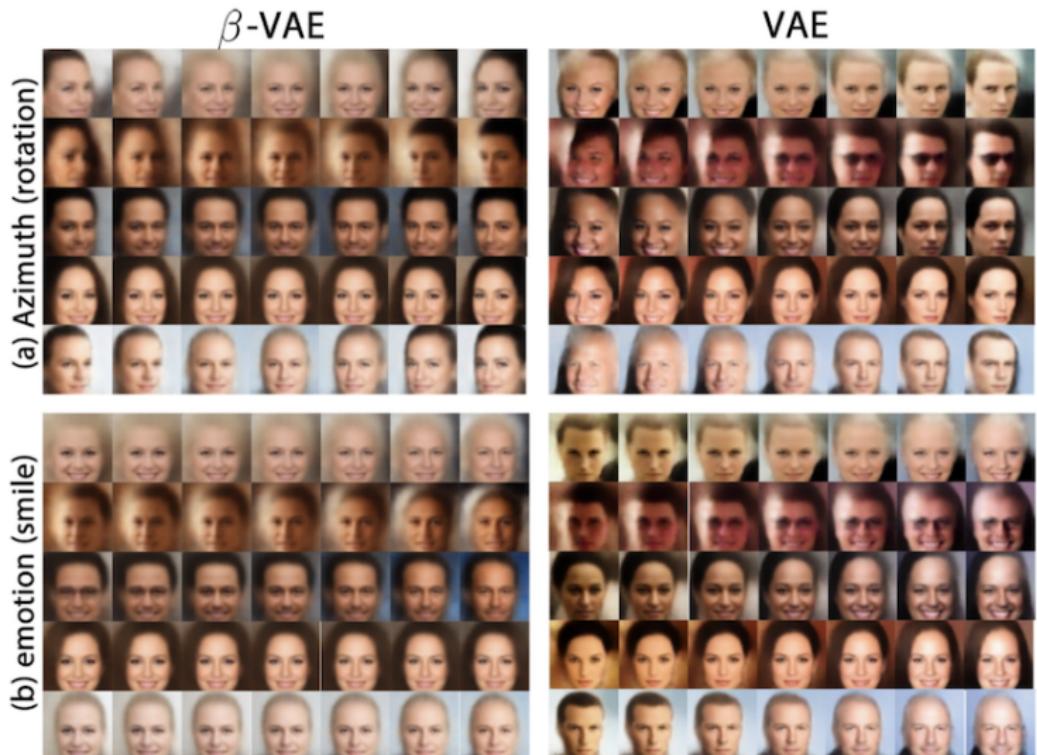
What do we get at  $\beta = 1$ ?

## Constrained optimization

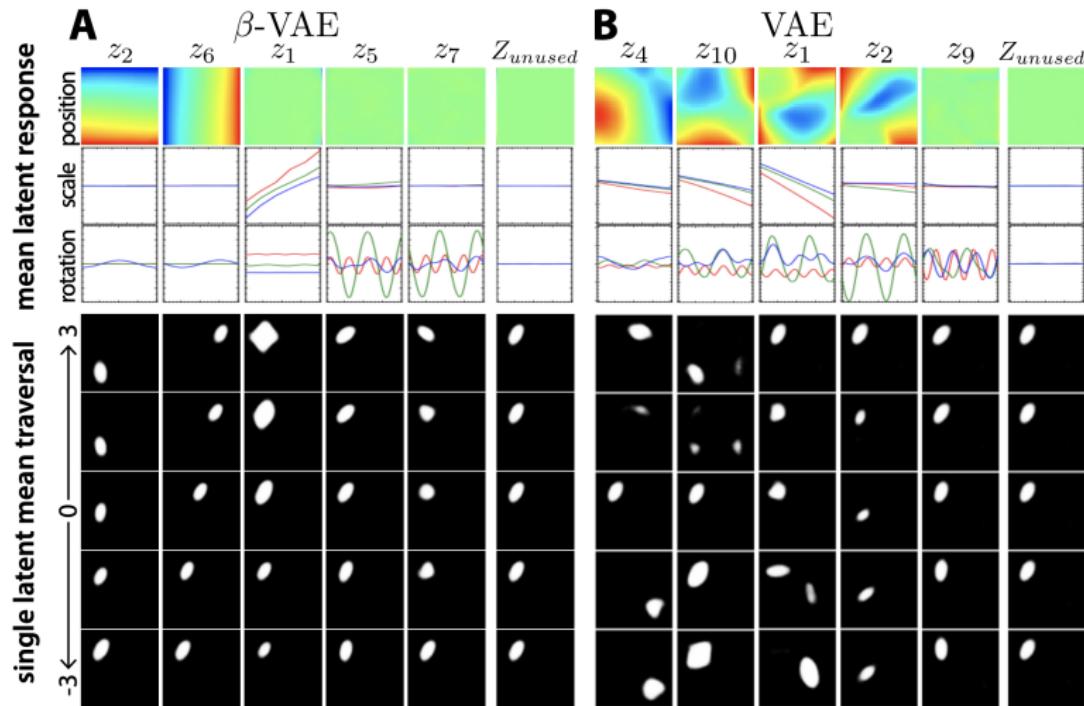
$$\max_{q, \theta} \mathbb{E}_{q(z|x)} \log p(x|z, \theta), \quad \text{subject to } KL(q(z|x)||p(z)) < \epsilon.$$

**Note:** It leads to poorer reconstructions and a loss of high frequency details.

# $\beta$ -VAE samples



# $\beta$ -VAE analysis



## $\beta$ -VAE

### ELBO

$$\mathcal{L}(q, \theta, \beta) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \log p(\mathbf{x}|\mathbf{z}, \theta) - \beta \cdot KL(q(\mathbf{z}|\mathbf{x})||p(\mathbf{z})).$$

### ELBO surgery

$$\frac{1}{n} \sum_{i=1}^n \mathcal{L}_i(q, \theta, \beta) = \underbrace{\frac{1}{n} \sum_{i=1}^n \mathbb{E}_{q(\mathbf{z}|\mathbf{x}_i)} \log p(\mathbf{x}_i|\mathbf{z}, \theta)}_{\text{Reconstruction loss}} - \underbrace{\beta \cdot \mathbb{I}_q[\mathbf{x}, \mathbf{z}]}_{\text{MI}} - \underbrace{\beta \cdot KL(q_{\text{agg}}(\mathbf{z})||p(\mathbf{z}))}_{\text{Marginal KL}}$$

### Minimization of MI

- ▶ It is not necessary and not desirable for disentanglement.
- ▶ It hurts reconstruction.

# $\beta$ -VAE

## Disentangling metric

1. Generate two sets of objects

$$\mathbf{x}_{li} \sim \text{Sim}(\mathbf{v}_{li}, \mathbf{w}_{li}); \quad \mathbf{x}_{lj} \sim \text{Sim}(\mathbf{v}_{lj}, \mathbf{w}_{lj}); \quad y_{ij} \sim U[1, d].$$

$$\mathbf{v}_{li} \sim p(\mathbf{v}); \quad \mathbf{v}_{lj} \sim p(\mathbf{v}) ([v_{li}]_y = [v_{lj}]_y); \quad \mathbf{w}_{li}, \mathbf{w}_{lj} \sim p(\mathbf{w}).$$

2. Find representations

$$q(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mu(\mathbf{x})|\sigma^2(\mathbf{x})); \quad \mathbf{z}_{li} = \mu(\mathbf{x}_{li}); \quad \mathbf{z}_{lj} = \mu(\mathbf{x}_{lj}).$$

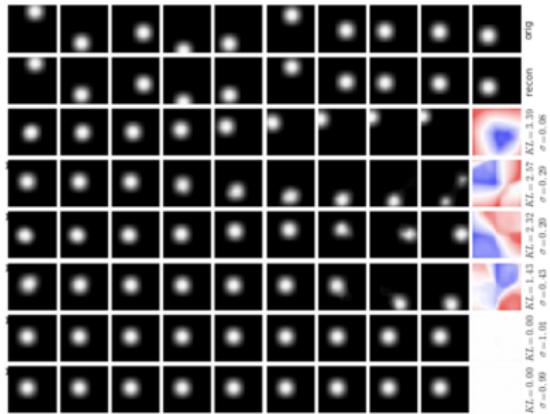
3. Use accuracy of classifier  $p(y|\mathbf{z}_{\text{diff}})$  with a low VC-dimension as metric of disentanglement

$$\mathbf{z}_{\text{diff}} = \frac{1}{L} \sum_{l=1}^L |\mathbf{z}_{li} - \mathbf{z}_{lj}|.$$

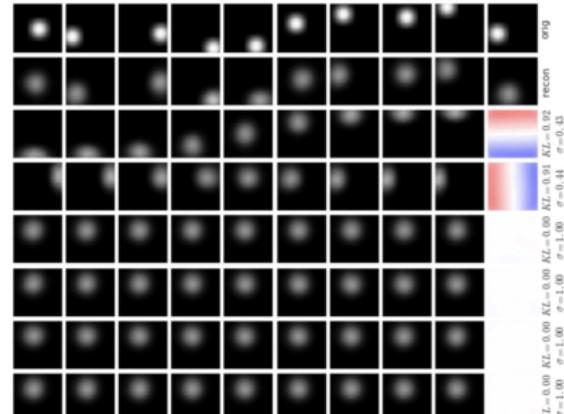
# $\beta$ -VAE

- ▶ **Top row:** original images.
- ▶ **Second row:** the corresponding reconstructions.
- ▶ **Remaining rows:** latent traversals ordered by KL divergence with the prior.
- ▶ **Heatmaps:** latent activations for each 2D position.

$\beta = 1$



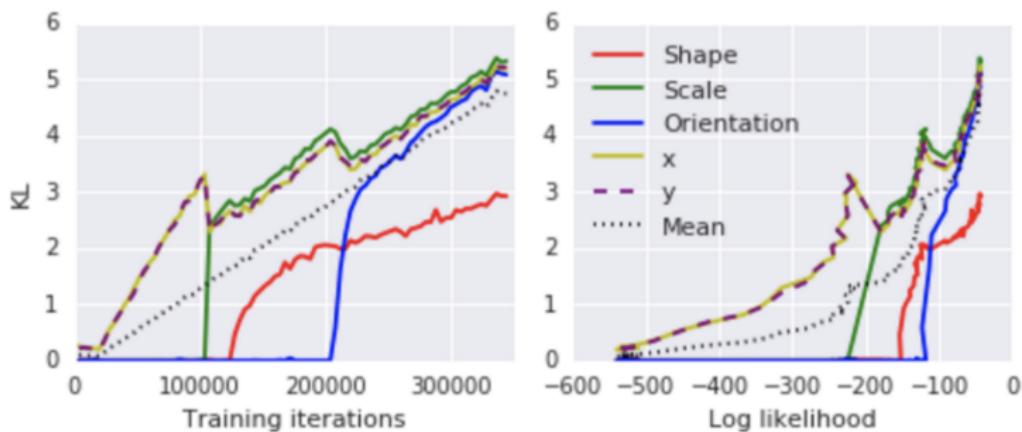
$\beta = 150$



# $\beta$ -VAE

## Controlled encoding capacity

$$\mathcal{L}(q, \theta, \beta) = \mathbb{E}_{q(z|x)} \log p(x|z, \theta) - [KL(q(z|x)||p(z)) - C].$$

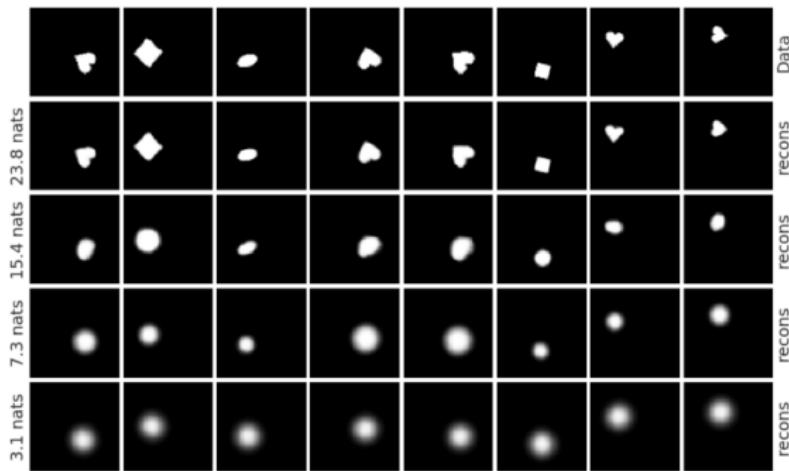


The early capacity is allocated to positional latents only, followed by a scale latent, then shape and orientation latents.

# $\beta$ -VAE

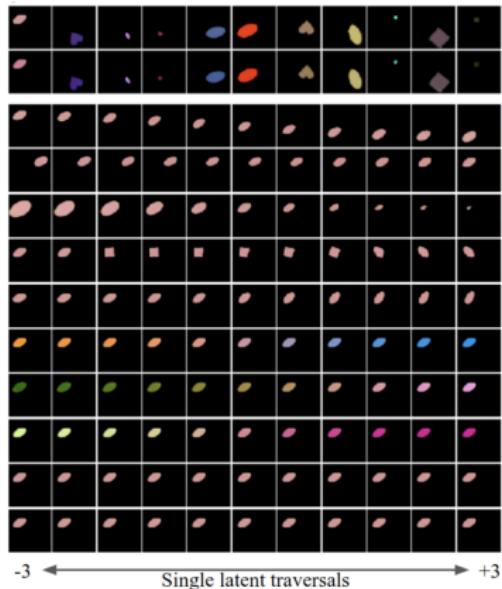
## Controlled encoding capacity

$$\mathcal{L}(q, \theta, \beta) = \mathbb{E}_{q(z|x)} \log p(x|z, \theta) - |KL(q(z|x)||p(z)) - C|.$$

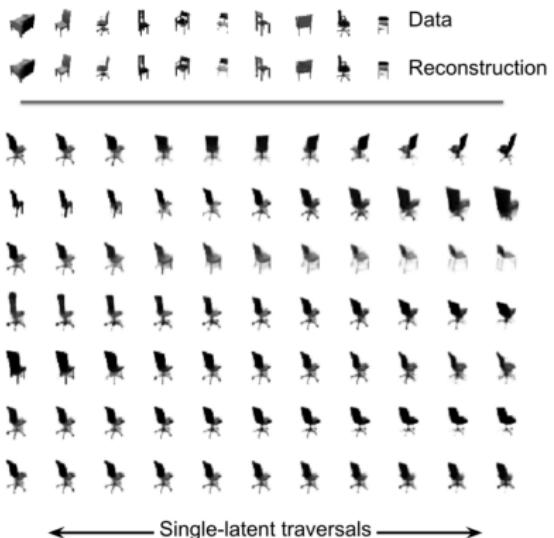


# $\beta$ -VAE

(a) Coloured dSprites



(b) 3D Chairs



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InfoGAN

$\beta$ -VAE

**DIP-VAE**

FactorVAE

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# DIP-VAE: disentangled posterior

Disentangled aggregated variational posterior

$$q_{\text{agg}}(\mathbf{z}) = \frac{1}{n} \sum_{i=1}^n q(\mathbf{z}|\mathbf{x}) = \prod_{j=1}^d q_{\text{agg}}(z_j)$$

DIP-VAE objective

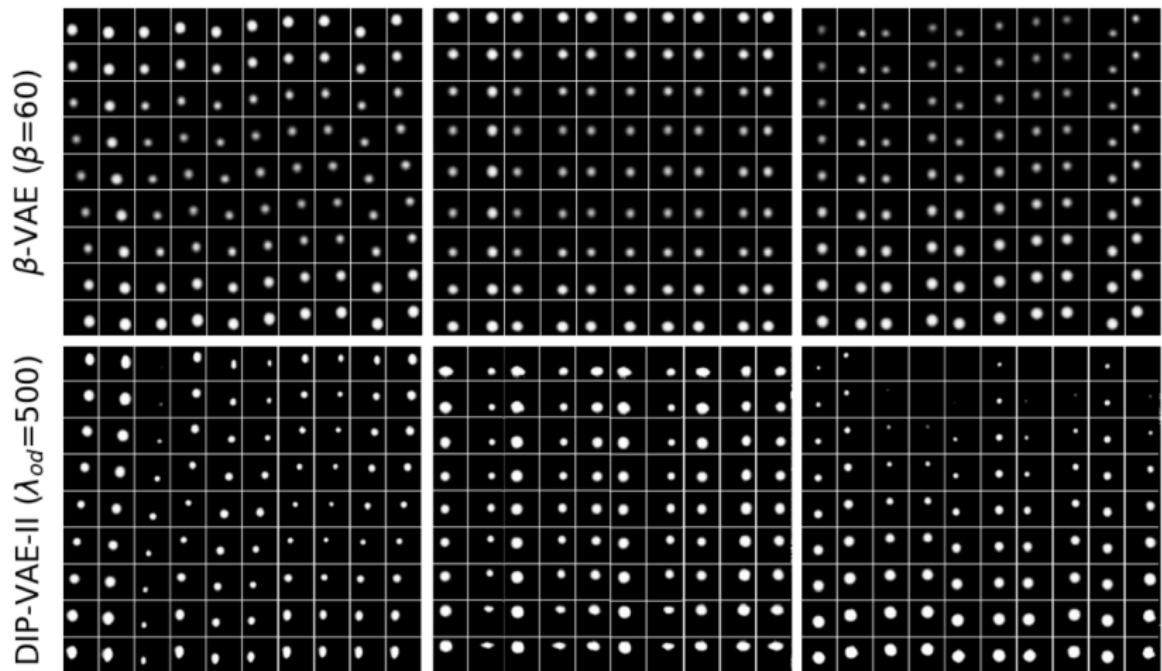
$$\begin{aligned}\mathcal{L}_{\text{DIP}}(q, \theta) &= \frac{1}{n} \sum_{i=1}^n \mathcal{L}_i(q, \theta) - \lambda \cdot KL(q_{\text{agg}}(\mathbf{z}) || p(\mathbf{z})) = \\ &= \underbrace{\frac{1}{n} \sum_{i=1}^n [\mathbb{E}_{q(\mathbf{z}|\mathbf{x}_i)} \log p(\mathbf{x}_i|\mathbf{z}, \theta)]}_{\text{Reconstruction loss}} - \underbrace{\mathbb{I}_q[\mathbf{x}, \mathbf{z}]}_{\text{MI}} - \underbrace{(1 + \lambda) \cdot KL(q_{\text{agg}}(\mathbf{z}) || p(\mathbf{z}))}_{\text{Marginal KL}}\end{aligned}$$

Marginal KL term is intractable.  $\Rightarrow$  Let match the moments of  $q_{\text{agg}}(\mathbf{z})$  and  $p(\mathbf{z})$ :

$$\text{cov}_{q_{\text{agg}}(\mathbf{z})}(\mathbf{z}) = \mathbb{E}_{q_{\text{agg}}(\mathbf{z})} \left[ (\mathbf{z} - \mathbb{E}_{q_{\text{agg}}(\mathbf{z})}(\mathbf{z}))(\mathbf{z} - \mathbb{E}_{q_{\text{agg}}(\mathbf{z})}(\mathbf{z}))^T \right].$$

# DIP-VAE: analysis

Reconstructions become better.



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## 7. Disentanglement

InfoGAN

$\beta$ -VAE

DIP-VAE

**FactorVAE**

Challenging Disentanglement Assumptions

8. GANs

9. FFJORD

10. Vector Quantized VAE-2

11. Feature Quantized GAN

# FactorVAE

Disentangled aggregated variational posterior

$$q(\mathbf{z}) = \frac{1}{n} \sum_{i=1}^n q(\mathbf{z}|\mathbf{x}) = \prod_{j=1}^d q(z_j)$$

Total correlation regularizer

$$\min KL(q(\mathbf{z}) || \prod_{j=1}^d q(z_j))$$

FactorVAE objective

$$\min_{\phi, \theta} \mathcal{L}(\phi, \theta) - \gamma \cdot KL(q(\mathbf{z}) || \prod_{j=1}^d q(z_j))$$

- ▶ The last term is intractable.
- ▶ FactorVAE uses density ratio trick for estimation.

## FactorVAE

Consider two distributions  $q_1(\mathbf{x})$ ,  $q_2(\mathbf{x})$  and probabilistic model

$$p(\mathbf{x}|y) = \begin{cases} q_1(\mathbf{x}), & \text{if } y = 1, \\ q_2(\mathbf{x}), & \text{if } y = 0, \end{cases} \quad y \sim \text{Bern}(0.5).$$

### Density ratio trick

$$\begin{aligned} \frac{q_1(\mathbf{x})}{q_2(\mathbf{x})} &= \frac{p(\mathbf{x}|y=1)}{p(\mathbf{x}|y=0)} = \frac{p(y=1|\mathbf{x})p(\mathbf{x})}{p(y=1)} \Big/ \frac{p(y=0|\mathbf{x})p(\mathbf{x})}{p(y=0)} = \\ &= \frac{p(y=1|\mathbf{x})}{p(y=0|\mathbf{x})} = \frac{p(y=1|\mathbf{x})}{1 - p(y=1|\mathbf{x})} = \frac{D(\mathbf{x})}{1 - D(\mathbf{x})} \end{aligned}$$

Here  $D(\mathbf{x})$  could be treated as a discriminator a model the output of which is a probability that  $\mathbf{x}$  is a sample from  $q_1(\mathbf{x})$  rather than from  $q_2(\mathbf{x})$ .

# FactorVAE

## FactorVAE objective

$$\min_{\theta, \phi} \text{ELBO}(\theta, \phi) - \gamma \cdot KL(q(\mathbf{z}) || \prod_{j=1}^d q(z_j))$$

## Total correlation regularizer

$$\begin{aligned} KL(q(\mathbf{z}) || \prod_{j=1}^d q(z_j)) &= KL(q(\mathbf{z}) || \bar{q}(\mathbf{z})) = \\ &= \mathbb{E}_{q(\mathbf{z})} \log \frac{q(\mathbf{z})}{\bar{q}(\mathbf{z})} \approx \mathbb{E}_{q(\mathbf{z})} \log \frac{D(\mathbf{z})}{1 - D(\mathbf{z})} \end{aligned}$$

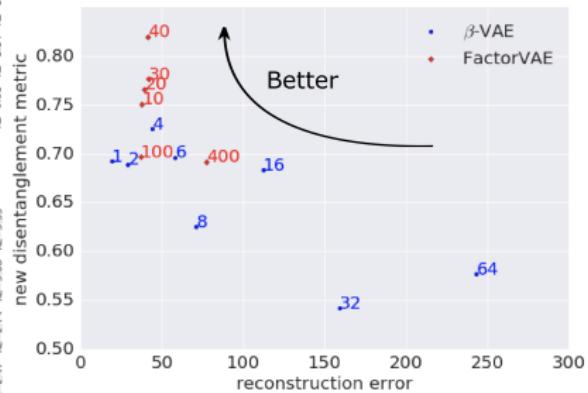
VAE and GAN are trained simultaneously.

# FactorVAE

$\beta$ -VAE ( $\beta = 8$ )



FactorVAE ( $\gamma = 10$ )



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# Challenging disentanglement assumptions

## Theorem

Let  $\mathbf{z}$  has density  $p(\mathbf{z}) = \prod_{i=1}^d p(z_i)$ . Then, there exists an **infinite** family of bijective functions  $f : \text{supp}(\mathbf{z}) \rightarrow \text{supp}(\mathbf{z})$ :

- ▶  $\frac{\partial f_i(\mathbf{z})}{\partial z_j} \neq 0$  for all  $i$  and  $j$  ( $\mathbf{z}$  and  $f(\mathbf{z})$  are completely entangled);
- ▶  $P(\mathbf{z} \leq \mathbf{u}) = P(f(\mathbf{z}) \leq \mathbf{u})$  for all  $\mathbf{u} \in \text{supp}(\mathbf{z})$ .

Consider a generative model with disentangled representation  $\mathbf{z}$ .

- ▶  $\exists \hat{\mathbf{z}} = f(\mathbf{z})$  where  $\hat{\mathbf{z}}$  is completely entangled with respect to  $\mathbf{z}$ .
- ▶ The disentanglement method cannot distinguish between the two equivalent generative models:

$$p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{z})p(\mathbf{z})d\mathbf{z} = \int p(\mathbf{x}|\hat{\mathbf{z}})p(\hat{\mathbf{z}})d\hat{\mathbf{z}}.$$

Theorem claims that unsupervised disentanglement learning is impossible for arbitrary generative models with a factorized prior.

# Challenging Disentanglement Assumptions

## Proof (1)

1. Consider the function  $g : \text{supp}(\mathbf{z}) \rightarrow [0, 1]^d$ :

$$g_i(\mathbf{u}) = P(z_i \leq u_i), \quad i = 1, \dots, d.$$

- ▶  $g$  is bijective (since  $p(\mathbf{z}) = \prod_{i=1}^d p(z_i)$ ).
  - ▶  $\frac{\partial g_i(\mathbf{u})}{\partial u_i} \neq 0$ , for all  $i$  and  $\frac{\partial g_i(\mathbf{u})}{\partial u_j} = 0$  for all  $i \neq j$ .
  - ▶  $g(\mathbf{z})$  is an independent  $d$ -dimensional uniform distribution.
2. Consider  $h : (0, 1]^d \rightarrow \mathbb{R}^d$

$$h_i(\mathbf{u}) = \psi^{-1}(u_i), \quad i = 1, \dots, d.$$

Here  $\psi$  denotes the CDF of a standard normal distribution.

- ▶  $h$  is bijective.
- ▶  $\frac{\partial h_i(\mathbf{u})}{\partial u_i} \neq 0$ , for all  $i$  and  $\frac{\partial h_i(\mathbf{u})}{\partial u_j} = 0$  for all  $i \neq j$ .
- ▶  $h(g(\mathbf{z}))$  is a  $d$ -dimensional standard normal distribution.

# Challenging Disentanglement Assumptions

## Proof (2)

Let  $\mathbf{A} \in \mathbb{R}^{d \times d}$  be an arbitrary orthogonal matrix with  $A_{ij} \neq 0$  for all  $i, j$ . The family of such matrices is infinite.

- ▶  $\mathbf{A}$  is orthogonal, it is invertible and thus defines a bijective linear operator.
- ▶  $\mathbf{A}h(g(\mathbf{z})) \in \mathbb{R}^d$  is hence an independent, multivariate standard normal distribution.
- ▶  $h^{-1}(\mathbf{A}h(g(\mathbf{z}))) \in \mathbb{R}^d$  is an independent  $d$ -dimensional uniform distribution.

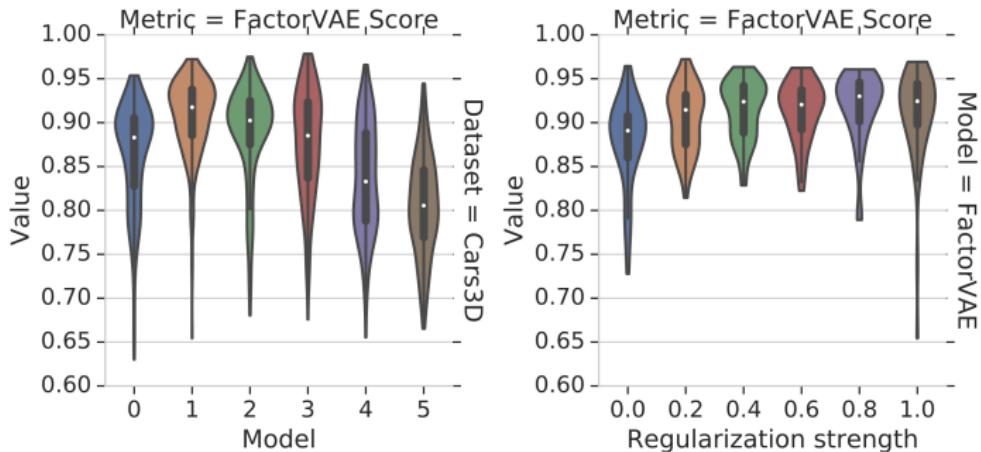
Define  $f : \text{supp}(\mathbf{z}) \rightarrow \text{supp}(\mathbf{z})$ :

$$f(\mathbf{u}) = g^{-1}(h^{-1}(\mathbf{A}h(g(\mathbf{z}))).$$

By definition  $f(\mathbf{z})$  has the same marginal distribution as  $\mathbf{z}$ :

$$P(\mathbf{z} \leq \mathbf{u}) = P(f(\mathbf{z}) \leq \mathbf{u}) \text{ and } \frac{\partial f_i(\mathbf{z})}{\partial z_j} \neq 0.$$

# Challenging disentanglement assumptions



	Dataset = Noisy-dSprites					
BetaVAE Score (A)	100	80	44	41	46	37
FactorVAE Score (B)	80	100	49	52	25	38
MIG (C)	44	49	100	76	6	42
DCI Disentanglement (D)	41	52	76	100	-8	38
Modularity (E)	46	25	6	-8	100	13
SAP (F)	37	38	42	38	13	100
	(A)	(B)	(C)	(D)	(E)	(F)

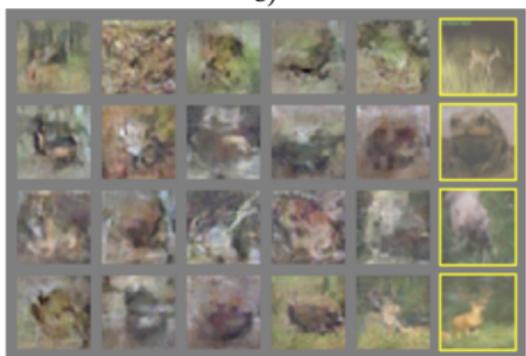
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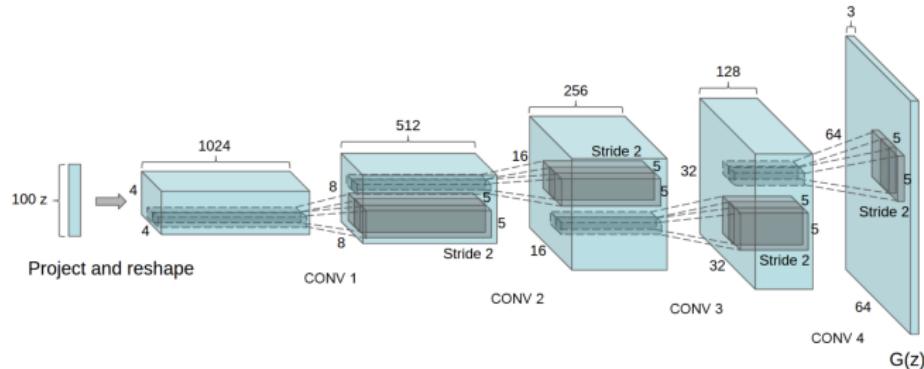
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# Vanilla GAN results



# Deep Convolutional GAN

## Architecture

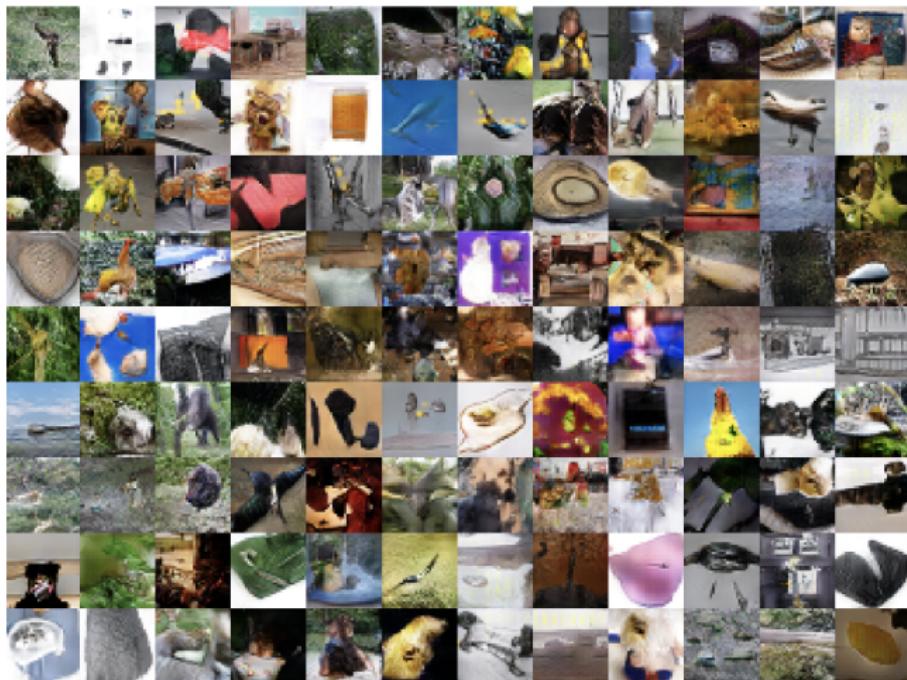


- ▶ Mean-pooling instead of max-pooling.
- ▶ Transposed convolutions in the generator for upsampling.
- ▶ Downsample with strided convolutions and average pooling.
- ▶ ReLU for generator, Leaky-ReLU (0.2) for discriminator.
- ▶ Output nonlinearity: tanh for Generator, sigmoid for discriminator.
- ▶ Batch Normalization used to prevent mode collapse (not applied at the output of  $G$  and input of  $D$ ).
- ▶ Adam: small LR = 2e-4; small momentum: 0.5, batch-size: 128.

*Radford A., Metz L., Chintala S. Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks, 2015*

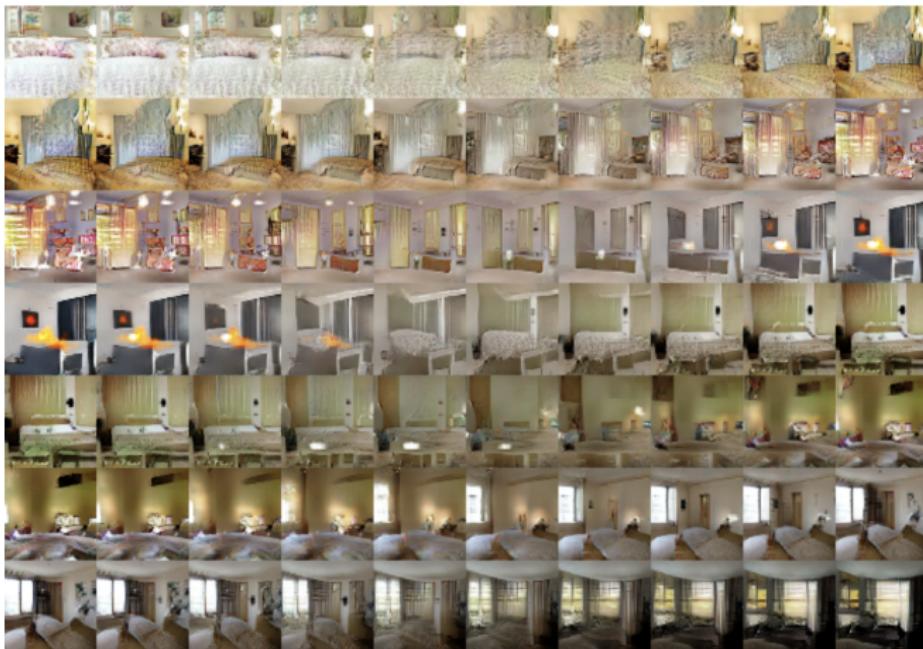
# Deep Convolutional GAN

## ImageNet samples



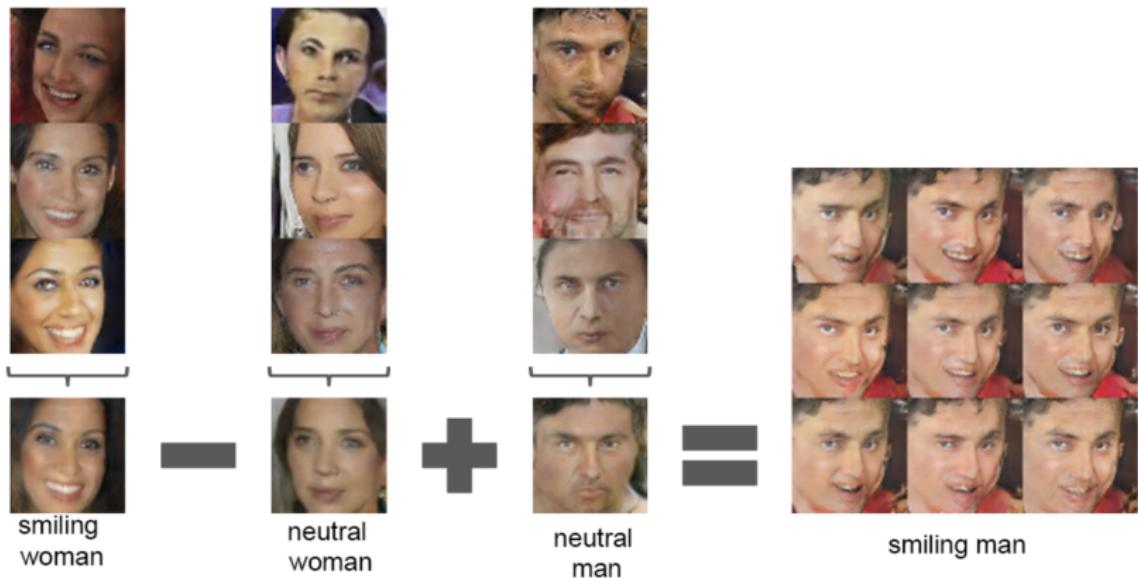
# Deep Convolutional GAN

## Smooth interpolations



# Deep Convolutional GAN

## Vector arithmetic



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# Improved techniques for training GANs

- ▶ Feature matching

$$\mathcal{L}_G = \|\mathbb{E}_{\pi(\mathbf{x})} \mathbf{d}(\mathbf{x}) - \mathbb{E}_{p(\mathbf{z})} \mathbf{d}(G(\mathbf{z}))\|_2^2$$

Here  $\mathbf{d}(\mathbf{x})$  – intermediate layer of discriminator. Matching the learned discriminator statistics instead of the output of the discriminator. Helps to avoid the vanishing gradients for sufficiently good discriminator.

- ▶ Historical averaging adds extra loss term for generator and discriminator losses

$$\|\boldsymbol{\theta} - \frac{1}{T} \sum_{t=1}^T \boldsymbol{\theta}_t\|_2^2.$$

Here  $\boldsymbol{\theta}_t$  – value of parameters at the previous step  $t$ . It allows to stabilize training procedure.

# Improved techniques for training GANs

- ▶ One-sided label smoothing. Instead of using one-hot labels in classification, use  $(1 - \alpha)$  for real data (the generated samples are not smoothed).

$$D^*(\mathbf{x}) = \frac{(1 - \alpha)\pi(\mathbf{x})}{\pi(\mathbf{x}) + p(\mathbf{x}|\theta)}$$

- ▶ Virtual batch normalization. BatchNorm makes samples within minibatch are highly correlated.



Use reference fixed batch to compute the normalization statistics. To avoid overfitting construct batch with the reference batch and the current sample.

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# Wasserstein GAN

---

**Algorithm 1** WGAN, our proposed algorithm. All experiments in the paper used the default values  $\alpha = 0.00005$ ,  $c = 0.01$ ,  $m = 64$ ,  $n_{\text{critic}} = 5$ .

---

**Require:** :  $\alpha$ , the learning rate.  $c$ , the clipping parameter.  $m$ , the batch size.  
 $n_{\text{critic}}$ , the number of iterations of the critic per generator iteration.

**Require:** :  $w_0$ , initial critic parameters.  $\theta_0$ , initial generator's parameters.

```
1: while  $\theta$  has not converged do
2:   for  $t = 0, \dots, n_{\text{critic}}$  do
3:     Sample  $\{x^{(i)}\}_{i=1}^m \sim \mathbb{P}_r$  a batch from the real data.
4:     Sample  $\{z^{(i)}\}_{i=1}^m \sim p(z)$  a batch of prior samples.
5:      $g_w \leftarrow \nabla_w [\frac{1}{m} \sum_{i=1}^m f_w(x^{(i)}) - \frac{1}{m} \sum_{i=1}^m f_w(g_\theta(z^{(i)}))]$ 
6:      $w \leftarrow w + \alpha \cdot \text{RMSProp}(w, g_w)$ 
7:      $w \leftarrow \text{clip}(w, -c, c)$ 
8:   end for
9:   Sample  $\{z^{(i)}\}_{i=1}^m \sim p(z)$  a batch of prior samples.
10:   $g_\theta \leftarrow -\nabla_\theta \frac{1}{m} \sum_{i=1}^m f_w(g_\theta(z^{(i)}))$ 
11:   $\theta \leftarrow \theta - \alpha \cdot \text{RMSProp}(\theta, g_\theta)$ 
12: end while
```

---

# Wasserstein GAN with Gradient Penalty

---

**Algorithm 1** WGAN with gradient penalty. We use default values of  $\lambda = 10$ ,  $n_{\text{critic}} = 5$ ,  $\alpha = 0.0001$ ,  $\beta_1 = 0$ ,  $\beta_2 = 0.9$ .

---

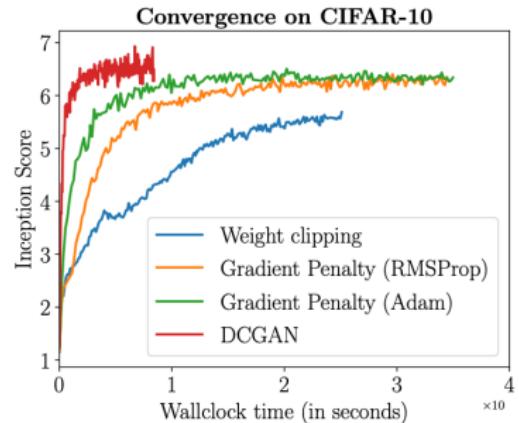
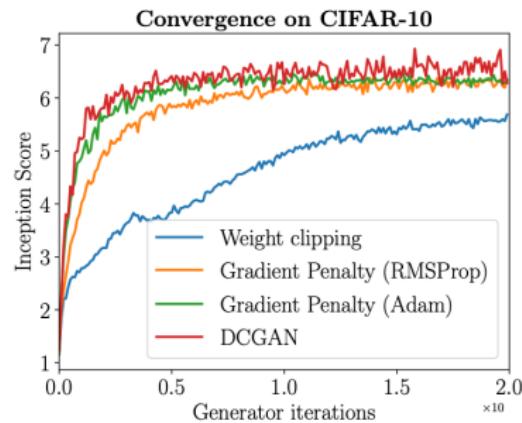
**Require:** The gradient penalty coefficient  $\lambda$ , the number of critic iterations per generator iteration  $n_{\text{critic}}$ , the batch size  $m$ , Adam hyperparameters  $\alpha, \beta_1, \beta_2$ .

**Require:** initial critic parameters  $w_0$ , initial generator parameters  $\theta_0$ .

```
1: while  $\theta$  has not converged do
2:   for  $t = 1, \dots, n_{\text{critic}}$  do
3:     for  $i = 1, \dots, m$  do
4:       Sample real data  $\mathbf{x} \sim \mathbb{P}_r$ , latent variable  $\mathbf{z} \sim p(\mathbf{z})$ , a random number  $\epsilon \sim U[0, 1]$ .
5:        $\tilde{\mathbf{x}} \leftarrow G_\theta(\mathbf{z})$ 
6:        $\hat{\mathbf{x}} \leftarrow \epsilon \mathbf{x} + (1 - \epsilon) \tilde{\mathbf{x}}$ 
7:        $L^{(i)} \leftarrow D_w(\tilde{\mathbf{x}}) - D_w(\mathbf{x}) + \lambda(\|\nabla_{\hat{\mathbf{x}}} D_w(\hat{\mathbf{x}})\|_2 - 1)^2$ 
8:     end for
9:      $w \leftarrow \text{Adam}(\nabla_w \frac{1}{m} \sum_{i=1}^m L^{(i)}, w, \alpha, \beta_1, \beta_2)$ 
10:   end for
11:   Sample a batch of latent variables  $\{\mathbf{z}^{(i)}\}_{i=1}^m \sim p(\mathbf{z})$ .
12:    $\theta \leftarrow \text{Adam}(\nabla_\theta \frac{1}{m} \sum_{i=1}^m -D_w(G_\theta(\mathbf{z})), \theta, \alpha, \beta_1, \beta_2)$ 
13: end while
```

---

# Wasserstein GAN with Gradient Penalty



## WGANGP convergence

Min. score	Only GAN	Only WGANGP	Both succeeded	Both failed
1.0	0	8	192	0
3.0	1	88	110	1
5.0	0	147	42	11
7.0	1	104	5	90
9.0	0	0	0	200

# Spectral Normalization GAN

---

**Algorithm 1** SGD with spectral normalization

---

- Initialize  $\tilde{\mathbf{u}}_l \in \mathcal{R}^{d_l}$  for  $l = 1, \dots, L$  with a random vector (sampled from isotropic distribution).
- For each update and each layer  $l$ :
  1. Apply power iteration method to a unnormalized weight  $W^l$ :

$$\tilde{\mathbf{v}}_l \leftarrow (W^l)^T \tilde{\mathbf{u}}_l / \| (W^l)^T \tilde{\mathbf{u}}_l \|_2 \quad (20)$$

$$\tilde{\mathbf{u}}_l \leftarrow W^l \tilde{\mathbf{v}}_l / \| W^l \tilde{\mathbf{v}}_l \|_2 \quad (21)$$

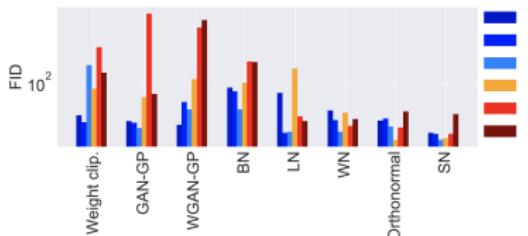
2. Calculate  $\bar{W}_{\text{SN}}$  with the spectral norm:

$$\bar{W}_{\text{SN}}^l(W^l) = W^l / \sigma(W^l), \text{ where } \sigma(W^l) = \tilde{\mathbf{u}}_l^T W^l \tilde{\mathbf{v}}_l \quad (22)$$

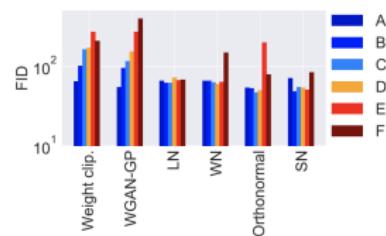
3. Update  $W^l$  with SGD on mini-batch dataset  $\mathcal{D}_M$  with a learning rate  $\alpha$ :

$$W^l \leftarrow W^l - \alpha \nabla_{W^l} \ell(\bar{W}_{\text{SN}}^l(W^l), \mathcal{D}_M) \quad (23)$$

---



(a) CIFAR-10



(b) STL-10

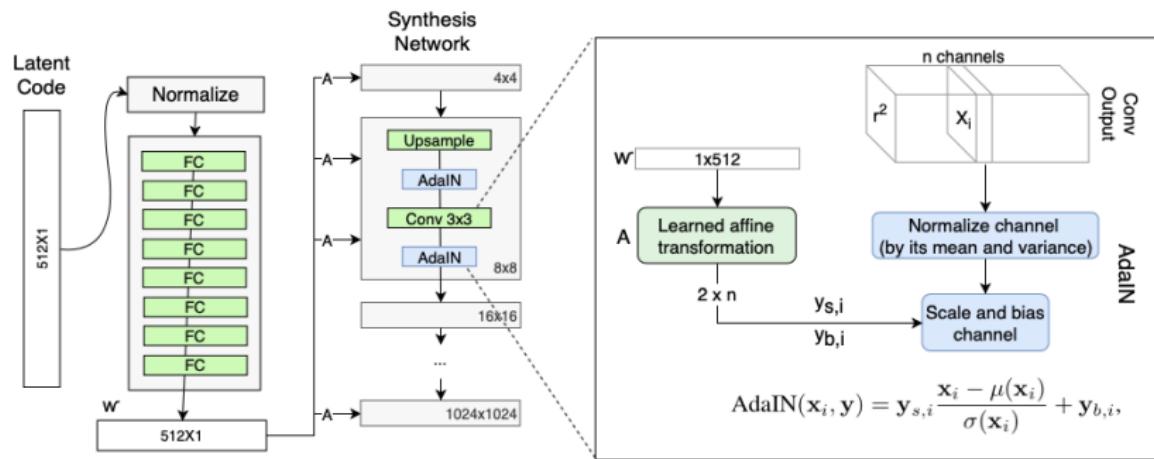
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# StyleGAN

## Step 2: Style modulation

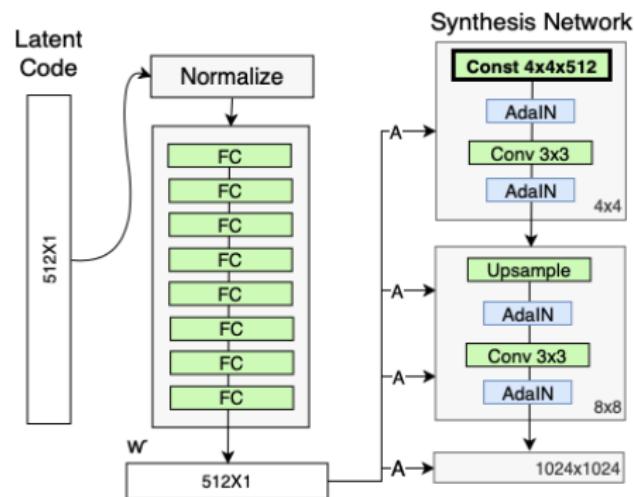
- ▶ Adaptive Instance Normalization transfers the  $\mathbf{w}$  vector to the synthesis Network.
- ▶ The module is added to each resolution to define the visual expression of the features.



# StyleGAN

## Step 3: Remove traditional input

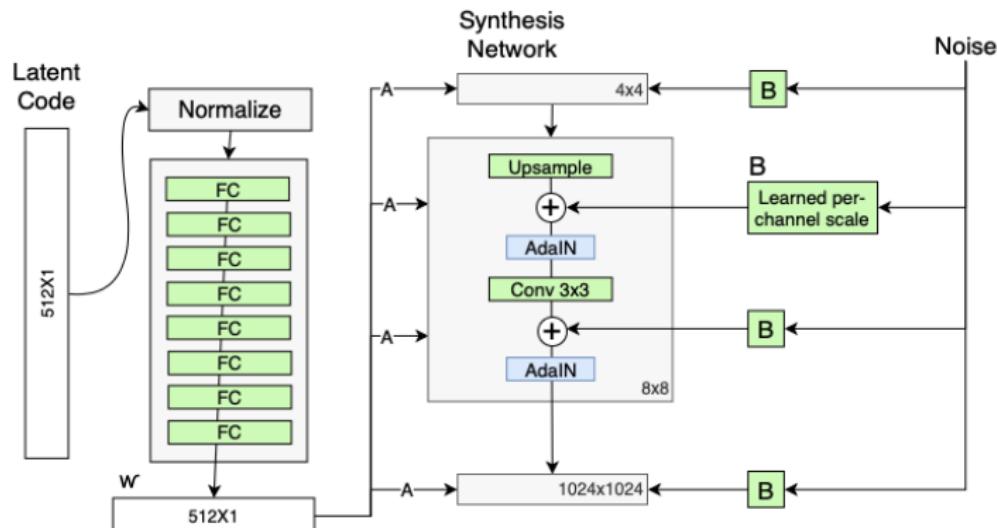
Mapping network provides stochasticity to different stages of the synthesis network. Input of the synthesis network is a trainable vector.



# StyleGAN

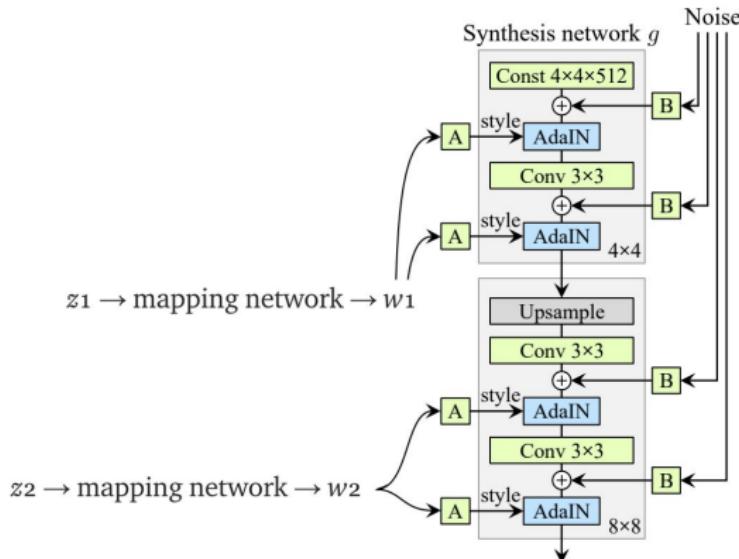
## Step 4: Stochastic variation

Inject random noise to add small aspects, such as freckles, exact placement of hairs, wrinkles, features which make the image more realistic and increase the variety of outputs.



# StyleGAN

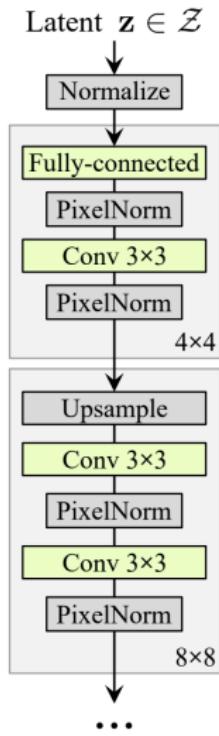
## Step 4: Style Mixing



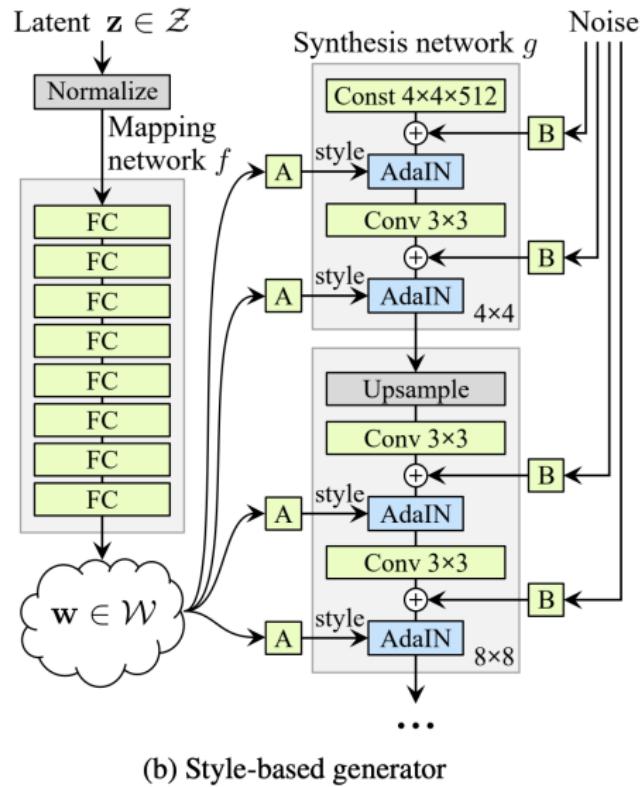
- ▶ Makes different levels of synthesis network to be independent.
- ▶ Allows to couple different styles.

Karras T., Laine S., Aila T. A Style-Based Generator Architecture for Generative Adversarial Networks, 2018

# StyleGAN

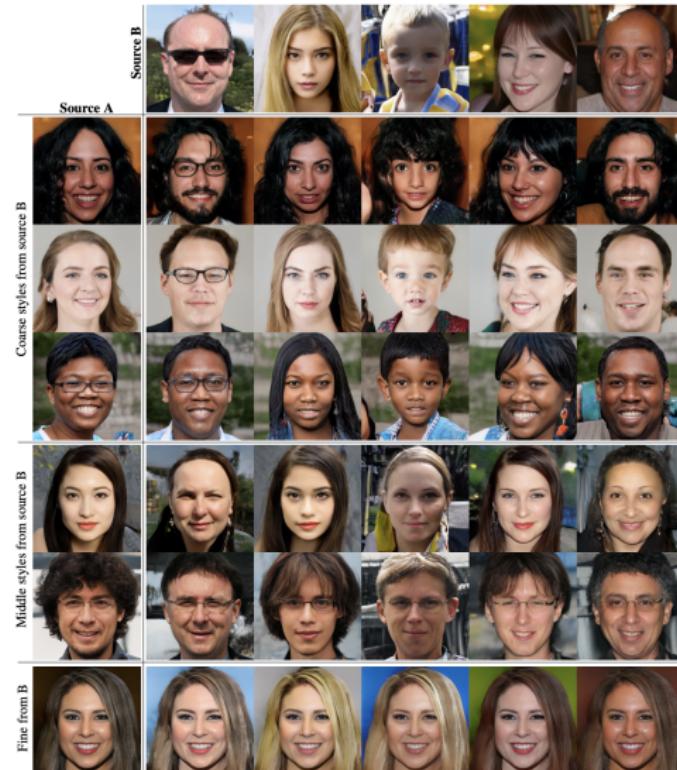


(a) Traditional



(b) Style-based generator

# StyleGAN



*Karras T., Laine S., Aila T. A Style-Based Generator Architecture for Generative Adversarial Networks, 2018*

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# Continuous Normalizing Flows

Forward transform + log-density

$$\begin{bmatrix} \mathbf{x} \\ \log p(\mathbf{x}|\boldsymbol{\theta}) \end{bmatrix} = \begin{bmatrix} \mathbf{z} \\ \log p(\mathbf{z}) \end{bmatrix} + \int_{t_0}^{t_1} \begin{bmatrix} f(\mathbf{z}(t), \boldsymbol{\theta}) \\ -\text{trace}\left(\frac{\partial f(\mathbf{z}(t), \boldsymbol{\theta})}{\partial \mathbf{z}(t)}\right) \end{bmatrix} dt.$$

- ▶ Discrete-in-time normalizing flows need invertible  $f$ . It costs  $O(d^3)$  to get determinant of Jacobian.
- ▶ Continuous-in-time flows require only smoothness of  $f$ . It costs  $O(d^2)$  to get trace of Jacobian.

It is possible to reduce cost from  $O(d^2)$  to  $O(d)$ !

Hutchinson's trace estimator

$$\text{trace}(A) = \mathbb{E}_{p(\epsilon)} \left[ \epsilon^T A \epsilon \right]; \quad \mathbb{E}[\epsilon] = 0; \quad \text{Cov}(\epsilon) = I.$$

FFJORD density estimation

$$\log p(\mathbf{z}(t_1)) = \log p(\mathbf{z}(t_0)) - \mathbb{E}_{p(\epsilon)} \int_{t_0}^{t_1} \left[ \epsilon^T \frac{\partial f}{\partial \mathbf{z}} \epsilon \right] dt.$$

Method		One-pass Sampling	Exact log-likelihood	Free-form Jacobian
Variational Autoencoders	Variational Autoencoders	✓	✗	✓
	Generative Adversarial Nets	✓	✗	✓
	Likelihood-based Autoregressive	✗	✓	✗
Change of Variables	Normalizing Flows	✓	✓	✗
	Reverse-NF, MAF, TAN	✗	✓	✗
	NICE, Real NVP, Glow, Planar CNF	✓	✓	✗
	<b>FFJORD</b>	✓	✓	✓

## Density estimation (forward KL)

	POWER	GAS	HEPMASS	MINIBOONE	BSDS300	MNIST	CIFAR10
Real NVP	-0.17	-8.33	18.71	13.55	-153.28	1.06*	3.49*
Glow	-0.17	-8.15	18.92	11.35	-155.07	1.05*	<b>3.35*</b>
<b>FFJORD</b>	<b>-0.46</b>	<b>-8.59</b>	<b>14.92</b>	<b>10.43</b>	<b>-157.40</b>	<b>0.99*</b> (1.05 <sup>†</sup> )	3.40*

## Flows for variational inference (reverse KL)

	MNIST	Omniglot	Frey Faces	Caltech Silhouettes
IAF	$84.20 \pm .17$	$102.41 \pm .04$	$4.47 \pm .05$	$111.58 \pm .38$
Sylvester	$83.32 \pm .06$	$99.00 \pm .04$	$4.45 \pm .04$	$104.62 \pm .29$
<b>FFJORD</b>	<b><math>82.82 \pm .01</math></b>	<b><math>98.33 \pm .09</math></b>	<b><math>4.39 \pm .01</math></b>	<b><math>104.03 \pm .43</math></b>

Grathwohl W. et al. FFJORD: Free-form Continuous Dynamics for Scalable Reversible Generative Models, 2018

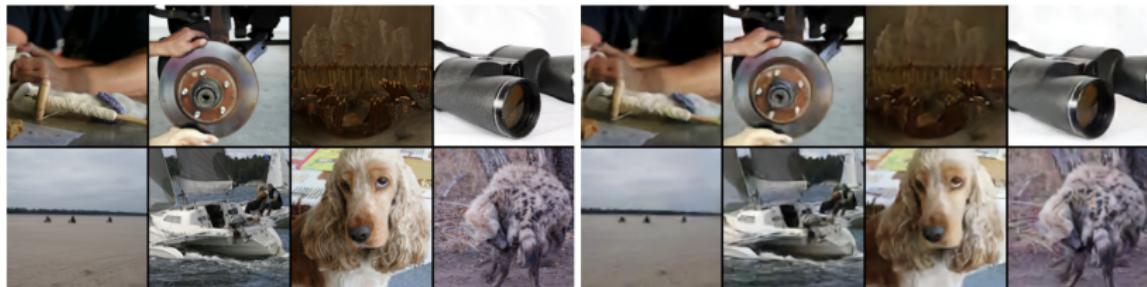
# Outline

1. Autoregressive models
2. Variational inference
3. VAE-related topics
4. Normalizing Flows
5. RevNet, i-RevNet
6. ELBO surgery
7. Disentanglement
8. GANs
9. FFJORD
10. Vector Quantized VAE-2
11. Feature Quantized GAN

# Vector Quantized VAE

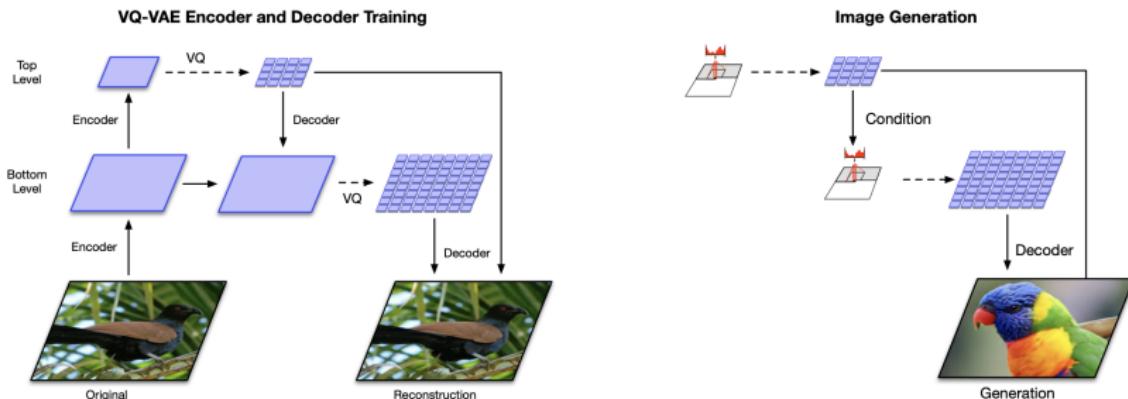
- ▶ The prior distribution over the discrete latents  $p(\hat{z})$  is a categorical distribution.
- ▶ It could be made autoregressive by depending on other  $\hat{z}$  in the feature map.
- ▶ While training the VQ-VAE, the prior is kept constant and uniform.
- ▶ After training, fit an autoregressive distribution (using PixelCNN) over  $\hat{z}$ .

## Samples



# Vector Quantized VAE-2

- ▶ Use multi-scale hierarchical model.
- ▶ Use autoregressive prior model in each scale of the hierarchy.
- ▶ Improve autoregressive prior (PixelSNAIL with self-attention in bottom layer, PixelCNN++ in bottom layer).
- ▶ Train the encoder and decoder at the first stage, train the priors at the second stage.



# Vector Quantized VAE-2

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**Algorithm 1** VQ-VAE training (stage 1)

**Require:** Functions  $E_{top}$ ,  $E_{bottom}$ ,  $D$ ,  $\mathbf{x}$   
(batch of training images)

- 1:  $\mathbf{h}_{top} \leftarrow E_{top}(\mathbf{x})$   
    ▷ quantize with top codebook eq 1
- 2:  $\mathbf{e}_{top} \leftarrow Quantize(\mathbf{h}_{top})$
- 3:  $\mathbf{h}_{bottom} \leftarrow E_{bottom}(\mathbf{x}, \mathbf{e}_{top})$   
    ▷ quantize with bottom codebook eq 1
- 4:  $\mathbf{e}_{bottom} \leftarrow Quantize(\mathbf{h}_{bottom})$
- 5:  $\hat{\mathbf{x}} \leftarrow D(\mathbf{e}_{top}, \mathbf{e}_{bottom})$   
    ▷ Loss according to eq 2
- 6:  $\theta \leftarrow Update(\mathcal{L}(\mathbf{x}, \hat{\mathbf{x}}))$

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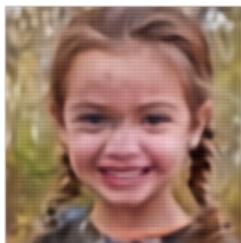
**Algorithm 2** Prior training (stage 2)

- 1:  $\mathbf{T}_{top}, \mathbf{T}_{bottom} \leftarrow \emptyset$                           ▷ training set
- 2: **for**  $\mathbf{x} \in$  training set **do**
- 3:      $\mathbf{e}_{top} \leftarrow Quantize(E_{top}(\mathbf{x}))$
- 4:      $\mathbf{e}_{bottom} \leftarrow Quantize(E_{bottom}(\mathbf{x}, \mathbf{e}_{top}))$
- 5:      $\mathbf{T}_{top} \leftarrow \mathbf{T}_{top} \cup \mathbf{e}_{top}$
- 6:      $\mathbf{T}_{bottom} \leftarrow \mathbf{T}_{bottom} \cup \mathbf{e}_{bottom}$
- 7: **end for**
- 8:  $p_{top} = TrainPixelCNN(\mathbf{T}_{top})$
- 9:  $p_{bottom} = TrainCondPixelCNN(\mathbf{T}_{bottom}, \mathbf{T}_{top})$

    ▷ Sampling procedure

- 10: **while** true **do**
- 11:      $\mathbf{e}_{top} \sim p_{top}$
- 12:      $\mathbf{e}_{bottom} \sim p_{bottom}(\mathbf{e}_{top})$
- 13:      $\mathbf{x} \leftarrow D(\mathbf{e}_{top}, \mathbf{e}_{bottom})$
- 14: **end while**

---

 $h_{top}$  $h_{top}, h_{middle}$  $h_{top}, h_{middle}, h_{bottom}$ 

Original

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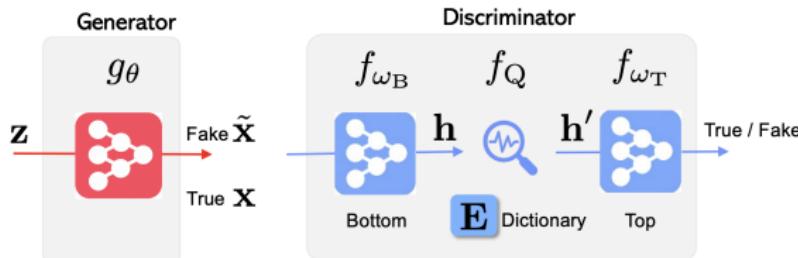
# Feature Quantized GAN

- ▶ GAN tries to find Nash equilibrium, minibatch training is unstable. GAN relies heavily on the minibatch statistics.
- ▶ Lots of feature matching strategies were proposed to stabilize the training.

## Feature quantized GAN discriminator

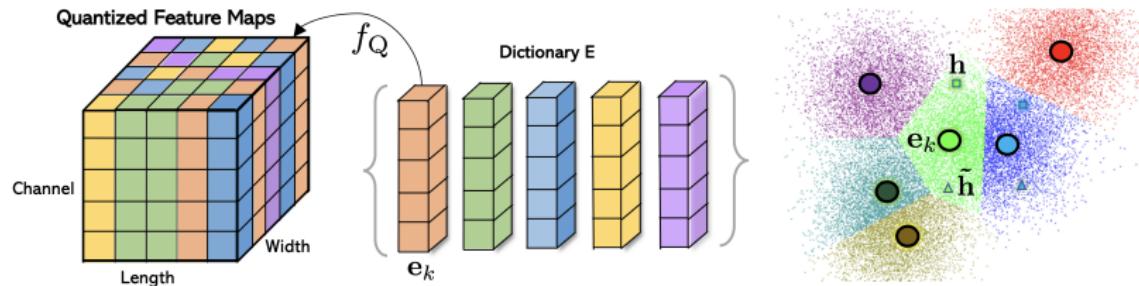
$$D(\mathbf{x}) = f_{\mathbf{w}_T} \circ f_{\mathbf{w}_B}(\mathbf{x}) \quad \Rightarrow \quad D(\mathbf{x}) = f_{\mathbf{w}_T} \circ f_Q \circ f_{\mathbf{w}_B}(\mathbf{x}).$$

Here  $f_Q$  is a vector quantization operation.

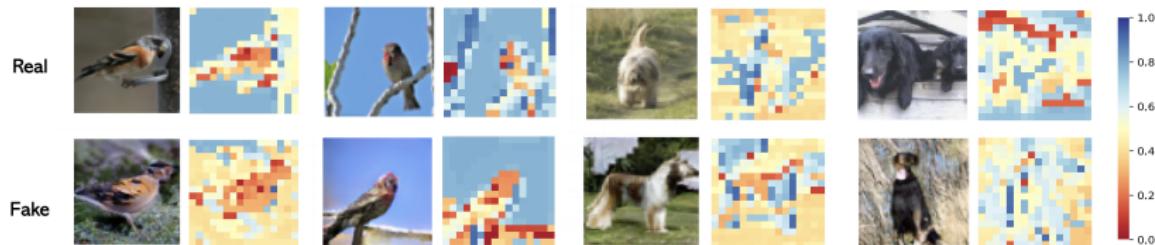


# Feature Quantized GAN

## Quantization procedure



## Quantized features



# Feature Quantized GAN

## ImageNet-1000

Models	64 × 64		128 × 128	
	FID* ↓ / IS* ↑		FID* ↓ / IS* ↑	
Half	TAC-GAN	-	23.75 / 28.86 $\pm$ 0.29 $^\ddagger$	
	BigGAN	12.75 / 21.84 $\pm$ 0.34	22.77 / 38.05 $\pm$ 0.79 $^\ddagger$	
256K	FQ-BigGAN	<b>12.62 / 21.99<math>\pm</math>0.32</b>	<b>19.11 / 41.92<math>\pm</math>1.15</b>	
	BigGAN	10.55 / 25.43 $\pm$ 0.15	14.88 / 63.03 $\pm$ 1.42 $^\dagger$	
	FQ-BigGAN	<b>9.67 / 25.96<math>\pm</math>0.24</b>	<b>13.77</b> / 54.36 $\pm$ 1.07	

## FFHQ

Resolution	32 <sup>2</sup>	64 <sup>2</sup>	128 <sup>2</sup>	1024 <sup>2</sup>
StyleGAN	3.28	4.82	6.33	5.24
FQ-StyleGAN	<b>3.01</b>	<b>4.36</b>	<b>5.98</b>	<b>4.89</b>

## Per class metrics for ImageNet

