

# Deep Generative Models

## Lecture 13

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## Recap of previous lecture

- ▶  $\mathcal{S}_\pi = \{\mathbf{x}_i\}_{i=1}^n \sim \pi(\mathbf{x})$  – real samples;
- ▶  $\mathcal{S}_p = \{\mathbf{x}_i\}_{i=1}^n \sim p(\mathbf{x}|\theta)$  – generated samples.

Embed samples using pretrained classifier network (as previously):

$$\mathcal{G}_\pi = \{\mathbf{g}_i\}_{i=1}^n, \quad \mathcal{G}_p = \{\mathbf{g}_i\}_{i=1}^n.$$

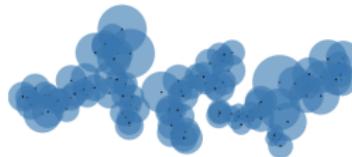
Define binary function:

$$f(\mathbf{g}, \mathcal{G}) = \begin{cases} 1, & \text{if exists } \mathbf{g}' \in \mathcal{G} : \|\mathbf{g} - \mathbf{g}'\|_2 \leq \|\mathbf{g} - \text{NN}_k(\mathbf{g}, \mathcal{G})\|_2; \\ 0, & \text{otherwise.} \end{cases}$$

$$\text{Precision}(\mathcal{G}_\pi, \mathcal{G}_p) = \frac{1}{n} \sum_{\mathbf{g} \in \mathcal{G}_p} f(\mathbf{g}, \mathcal{G}_\pi); \quad \text{Recall}(\mathcal{G}_\pi, \mathcal{G}_p) = \frac{1}{n} \sum_{\mathbf{g} \in \mathcal{G}_\pi} f(\mathbf{g}, \mathcal{G}_p).$$



(a) True manifold



(b) Approx. manifold

## Recap of previous lecture



- ▶ **Self-Attention GAN** allows to make huge receptive field and reduce convolution inductive bias.
- ▶ **BigGAN** shows that large batch size increase model quality gradually.
- ▶ **Progressive Growing GAN** starts from a low resolution, adds new layers that model fine details as training progresses.
- ▶ **StyleGAN** introduces mapping network to get more disentangled latent representation.

## Recap of previous lecture

### ELBO objective

$$\mathcal{L}(\phi, \theta) = \mathbb{E}_{q(z|x, \phi)} [\log p(x|z, \theta) + \log p(z) - \log q(z|x, \phi)] \rightarrow \max_{\phi, \theta}.$$

What is the problem to make the variational posterior model an **implicit** model?

- ▶ The third term requires the ability to calculate the value of  $q(z|x, \phi)$ .
- ▶ We could join second and third terms:

$$\mathbb{E}_{q(z|x, \phi)} \log \frac{p(z)}{q(z|x, \phi)} = \mathbb{E}_{q(z|x, \phi)} \log \frac{p(z)\pi(x)}{q(z|x, \phi)\pi(x)}.$$

- ▶ We have to estimate density ratio

$$r(x, z) = \frac{q_1(x, z)}{q_2(x, z)} = \frac{p(z)\pi(x)}{q(z|x, \phi)\pi(x)}.$$

## Recap of previous lecture

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

## Adversarial Variational Bayes

$$\max_D \left[ \mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \log D(\mathbf{x}, \mathbf{z}) + \mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{p(\mathbf{z})} \log(1 - D(\mathbf{x}, \mathbf{z})) \right]$$

# Neural ODE

Consider Ordinary Differential Equation

$$\frac{dz(t)}{dt} = f(z(t), \theta); \quad \text{with initial condition } z(t_0) = z_0.$$

$$z(t_1) = \int_{t_0}^{t_1} f(z(t), \theta) dt + z_0 = \text{ODESolve}(z(t_0), f, t_0, t_1, \theta).$$

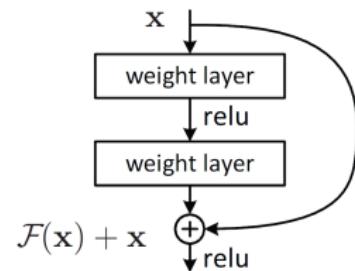
Euler update step

$$\frac{z(t + \Delta t) - z(t)}{\Delta t} = f(z(t), \theta) \Rightarrow z(t + \Delta t) = z(t) + \Delta t f(z(t), \theta).$$

Residual block

$$z_{t+1} = z_t + f(z_t, \theta)$$

- ▶ It is equivalent to Euler update step for solving ODE with  $\Delta t = 1$ !
- ▶ Euler update step is unstable and trivial.  
There are more sophisticated methods.



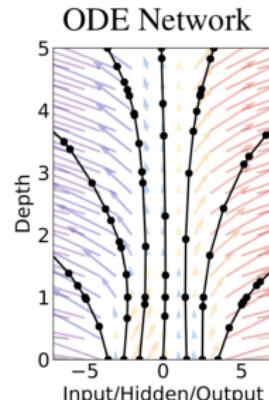
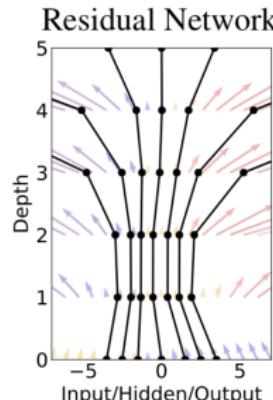
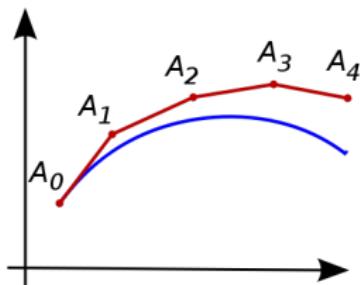
# Neural ODE

## Residual block

$$\mathbf{z}_{t+1} = \mathbf{z}_t + f(\mathbf{z}_t, \theta).$$

In the limit of adding more layers and taking smaller steps, we parameterize the continuous dynamics of hidden units using an ODE specified by a neural network:

$$\frac{d\mathbf{z}(t)}{dt} = f(\mathbf{z}(t), t, \theta); \quad \mathbf{z}(t_0) = \mathbf{x}; \quad \mathbf{z}(t_1) = \mathbf{y}.$$



# Neural ODE

## Forward pass (loss function)

$$\begin{aligned} L(\mathbf{y}) &= L(\mathbf{z}(t_1)) = L \left( \mathbf{z}(t_0) + \int_{t_0}^{t_1} f(\mathbf{z}(t), \theta) dt \right) \\ &= L(\text{ODESolve}(\mathbf{z}(t_0), f, t_0, t_1, \theta)) \end{aligned}$$

**Note:** ODESolve could be any method (Euler step, Runge-Kutta methods).

## Backward pass (gradients computation)

For fitting parameters we need gradients:

$$\mathbf{a}_\mathbf{z}(t) = \frac{\partial L(\mathbf{y})}{\partial \mathbf{z}(t)}; \quad \mathbf{a}_\theta(t) = \frac{\partial L(\mathbf{y})}{\partial \theta(t)}.$$

In theory of optimal control these functions called **adjoint** functions. They show how the gradient of the loss depends on the hidden state  $\mathbf{z}(t)$  and parameters  $\theta$ .

# Neural ODE

## Adjoint functions

$$\mathbf{a}_z(t) = \frac{\partial L(\mathbf{y})}{\partial \mathbf{z}(t)}; \quad \mathbf{a}_{\theta}(t) = \frac{\partial L(\mathbf{y})}{\partial \theta(t)}.$$

## Theorem (Pontryagin)

$$\frac{d\mathbf{a}_z(t)}{dt} = -\mathbf{a}_z(t)^T \cdot \frac{\partial f(\mathbf{z}(t), \theta)}{\partial \mathbf{z}}; \quad \frac{d\mathbf{a}_{\theta}(t)}{dt} = -\mathbf{a}_z(t)^T \cdot \frac{\partial f(\mathbf{z}(t), \theta)}{\partial \theta}.$$

Do we know any initial condition?

## Solution for adjoint function

$$\frac{\partial L}{\partial \theta(t_0)} = \mathbf{a}_{\theta}(t_0) = - \int_{t_1}^{t_0} \mathbf{a}_z(t)^T \frac{\partial f(\mathbf{z}(t), \theta)}{\partial \theta(t)} dt$$

$$\frac{\partial L}{\partial \mathbf{z}(t_0)} = \mathbf{a}_z(t_0) = - \int_{t_1}^{t_0} \mathbf{a}_z(t)^T \frac{\partial f(\mathbf{z}(t), \theta)}{\partial \mathbf{z}(t)} dt$$

**Note:** These equations are solved back in time.

# Neural ODE

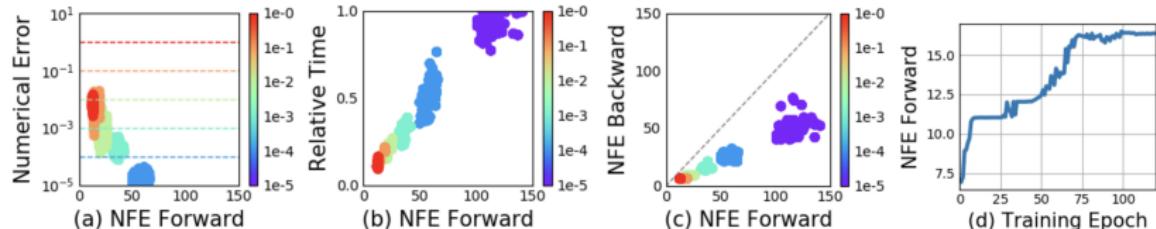
## Forward pass

$$\mathbf{z}(t_1) = \int_{t_0}^{t_1} f(\mathbf{z}(t), \theta) dt + \mathbf{z}_0 \quad \Rightarrow \quad \text{ODE Solver}$$

## Backward pass

$$\left. \begin{aligned} \frac{\partial L}{\partial \theta(t_0)} &= \mathbf{a}_\theta(t_0) = - \int_{t_1}^{t_0} \mathbf{a}_z(t)^\top \frac{\partial f(\mathbf{z}(t), \theta)}{\partial \theta(t)} dt \\ \frac{\partial L}{\partial \mathbf{z}(t_0)} &= \mathbf{a}_z(t_0) = - \int_{t_1}^{t_0} \mathbf{a}_z(t)^\top \frac{\partial f(\mathbf{z}(t), \theta)}{\partial \mathbf{z}(t)} dt \\ \mathbf{z}(t_0) &= - \int_{t_1}^{t_0} f(\mathbf{z}(t), \theta) dt + \mathbf{z}_1. \end{aligned} \right\} \Rightarrow \text{ODE Solver}$$

**Note:** This transformation is a generalization of usual backprop.



# Continuous Normalizing Flows

## Discrete Normalizing Flows

$$\mathbf{z}_{t+1} = f(\mathbf{z}_t, \theta); \quad \log p(\mathbf{z}_{t+1}) = \log p(\mathbf{z}_t) - \log \left| \det \frac{\partial f(\mathbf{z}_t, \theta)}{\partial \mathbf{z}_t} \right|.$$

Continuous-in-time dynamic transformation

$$\frac{d\mathbf{z}(t)}{dt} = f(\mathbf{z}(t), \theta).$$

Assume that function  $f$  is uniformly Lipschitz continuous in  $\mathbf{z}$  and continuous in  $t$ . From Picard's existence theorem, it follows that the above ODE has a **unique solution**.

Forward and inverse transforms

$$\mathbf{x} = \mathbf{z}(t_1) = \mathbf{z}(t_0) + \int_{t_0}^{t_1} f(\mathbf{z}(t), \theta) dt$$

$$\mathbf{z} = \mathbf{z}(t_0) = \mathbf{z}(t_1) + \int_{t_1}^{t_0} f(\mathbf{z}(t), \theta) dt$$

# Continuous Normalizing Flows

To train this flow we have to get the way to calculate the density  $p(\mathbf{z}(t))$ .

## Theorem

if function  $f$  is uniformly Lipschitz continuous in  $\mathbf{z}$  and continuous in  $t$ , then

$$\frac{\partial \log p(\mathbf{z}(t))}{\partial t} = -\text{trace}\left(\frac{\partial f(\mathbf{z}(t), \theta)}{\partial \mathbf{z}(t)}\right).$$

**Note:** Unlike discrete-in-time flows, the function  $f$  does not need to be bijective, because uniqueness guarantees that the entire transformation is automatically bijective.

## Density evaluation

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

**Adjoint** method is used to integral evaluation.

# 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  $O(d)$ !

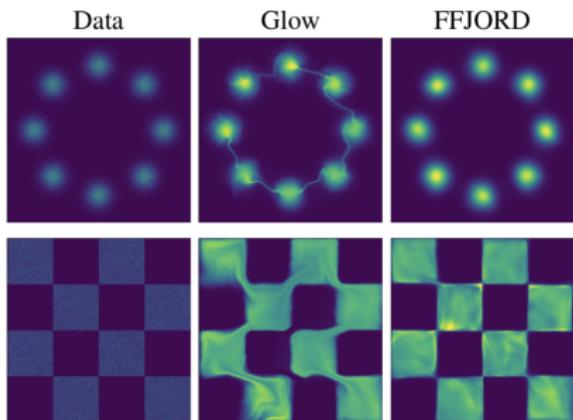
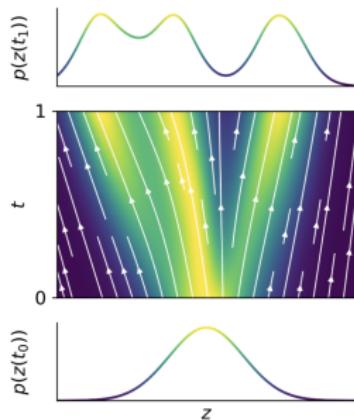
Hutchinson's trace estimator

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

FFJORD density estimation

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

# FFJORD



	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>	✓	✓	✓

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

# FFJORD

## Density estimation (forward KL)

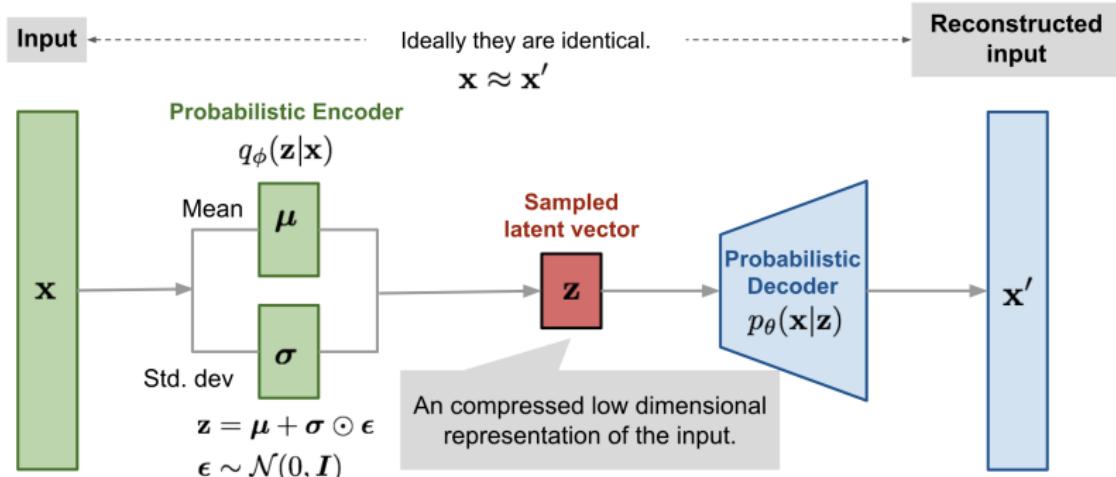
	POWER	GAS	HEPMASS	MINIBOONE	BSDS300	MNIST	CIFAR10
Real NVP	-0.17	-8.33	18.71	13.55	-153.28	1.06*	3.49*
Glow	-0.17	-8.15	18.92	11.35	-155.07	1.05*	<b>3.35*</b>
FFJORD	<b>-0.46</b>	<b>-8.59</b>	<b>14.92</b>	<b>10.43</b>	<b>-157.40</b>	<b>0.99*</b> (1.05 <sup>†</sup> )	3.40*
MADE	3.08	-3.56	20.98	15.59	-148.85	2.04	5.67
MAF	-0.24	-10.08	17.70	11.75	-155.69	1.89	4.31
TAN	-0.48	-11.19	15.12	11.01	-157.03	-	-
MAF-DDSF	-0.62	-11.96	15.09	8.86	-157.73	-	-

## Flows for variational inference (reverse KL)

	MNIST	Omniglot	Frey Faces	Caltech Silhouettes
No Flow	$86.55 \pm .06$	$104.28 \pm .39$	$4.53 \pm .02$	$110.80 \pm .46$
Planar	$86.06 \pm .31$	$102.65 \pm .42$	$4.40 \pm .06$	$109.66 \pm .42$
IAF	$84.20 \pm .17$	$102.41 \pm .04$	$4.47 \pm .05$	$111.58 \pm .38$
Sylvester	$83.32 \pm .06$	$99.00 \pm .04$	$4.45 \pm .04$	$104.62 \pm .29$
FFJORD	<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

# Discrete VAE



- ▶ Previous VAE models had **continuous** latent variables  $z$ .
- ▶ **Discrete** representations  $z$  are potentially a more natural fit for many of the modalities.
- ▶ Powerful autoregressive models (like PixelCNN) have been developed for modelling distributions over discrete variables.

# Discrete VAE

If  $\mathbf{z}$  is a discrete random variable we cannot differentiate through it.

## Gumbel-Max trick

Let  $G_k \sim \text{Gumbel}$  for  $k = 1, \dots, K$ , i.e.  $G = -\log(\log u)$ ,  $u \sim \text{Uniform}[0, 1]$ . Then a discrete random variable

$$z = \arg \max_k (\log \pi_k + G_k)$$

has a categorical distribution  $z \sim \text{Categorical}(\boldsymbol{\pi})$  ( $P(z = k) = \pi_k$ ).

**Problem:** We still have non-differentiable  $\arg \max$  operation.

## Gumbel-Softmax relaxation

$$z_k = \frac{\exp((\log \pi_k + G_k)/\tau)}{\sum_{j=1}^K \exp((\log \pi_j + G_j)/\tau)}, \quad k = 1, \dots, K.$$

Here  $\tau$  is a temperature parameter.

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*Maddison C. J., Mnih A., Teh Y. W. The Concrete distribution: A continuous relaxation of discrete random variables, 2016*

*Jang E., Gu S., Poole B. Categorical reparameterization with Gumbel-Softmax, 2016*

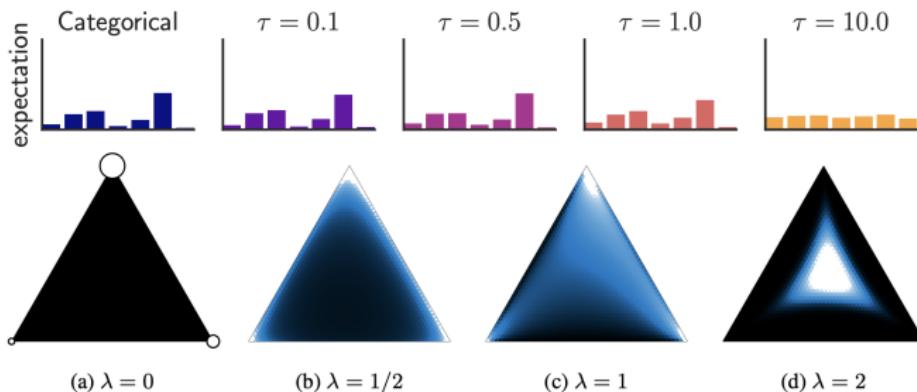
# Discrete VAE

## Gumbel-Softmax relaxation

Concrete distribution = continuous + discrete

$$z_k = \frac{\exp((\log \pi_k + G_k)/\tau)}{\sum_{j=1}^K \exp((\log \pi_j + G_j)/\tau)}, \quad k = 1, \dots, K.$$

Here  $\tau$  is a temperature parameter. Now we have differentiable operation.



Maddison C. J., Mnih A., Teh Y. W. *The Concrete distribution: A continuous relaxation of discrete random variables*, 2016

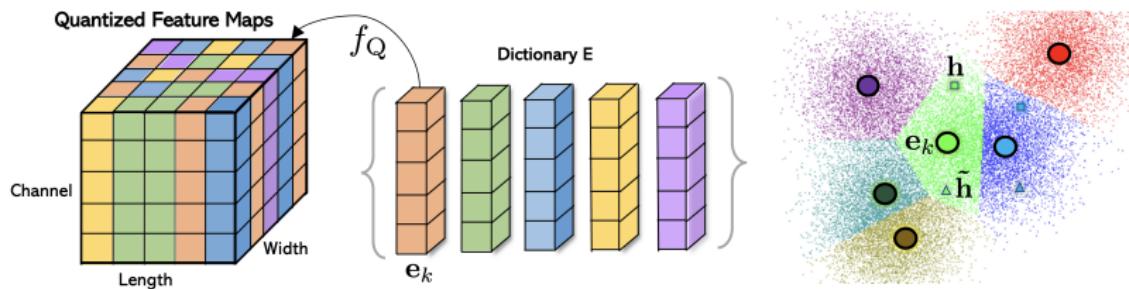
Jang E., Gu S., Poole B. *Categorical reparameterization with Gumbel-Softmax*, 2016

# Vector Quantized VAE

- ▶ Define dictionary space  $\{\mathbf{e}_k\}_{k=1}^K$ , where  $\mathbf{e}_k \in \mathbb{R}^C$ ,  $K$  is the size of the dictionary.
- ▶ Let  $\mathbf{z} = \text{NN}_e(\mathbf{x}) \in \mathbb{R}^{W \times H \times C}$  be an encoder output.
- ▶ Quantized representation  $\mathbf{z}_q \in \mathbb{R}^{W \times H \times C}$  is defined by a nearest neighbour look-up using the shared dictionary space for each of  $W \times H$  spatial locations

$$[\mathbf{z}_q]_{ij} = \mathbf{e}_{k^*}, \quad \text{where } k^* = \arg \min_k \|[\mathbf{z}_e]_{ij} - \mathbf{e}_k\|.$$

## Quantization procedure



## Vector Quantized VAE

Define VAE latent variable  $\hat{\mathbf{z}} \in \mathbb{R}^{W \times H}$  with prior distribution  $p(\hat{\mathbf{z}}) = \text{Uniform}\{1, \dots, K\}$  and variational posterior distribution

$$q(\hat{\mathbf{z}}|\mathbf{x}) = \prod_{i=1}^W \prod_{j=1}^H q(\hat{z}_{ij}|\mathbf{x})$$

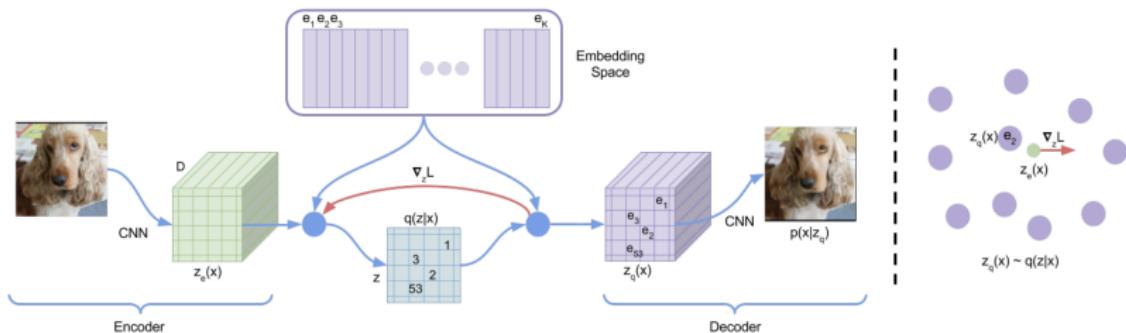
$$q(\hat{z}_{ij} = k^*|\mathbf{x}) = \begin{cases} 1, & \text{for } k^* = \arg \min_k \|[\mathbf{z}_e]_{ij} - \mathbf{e}_k\| \\ 0, & \text{otherwise.} \end{cases}$$

## ELBO objective

$$\mathcal{L}(\phi, \theta) = \mathbb{E}_{q(\hat{\mathbf{z}}|\mathbf{x}, \phi)} \log p(\mathbf{x}|\hat{\mathbf{z}}, \theta)] - KL(q(\hat{\mathbf{z}}|\mathbf{x})||p(\hat{\mathbf{z}})) \rightarrow \max_{\phi, \theta} .$$

- ▶ VAE proposal distribution  $q(z|\mathbf{x})$  is deterministic.
- ▶  $KL(q(\hat{\mathbf{z}}|\mathbf{x})||p(\hat{\mathbf{z}}))$  term in ELBO is constant (equals to  $\log K$ ).

# Vector Quantized VAE



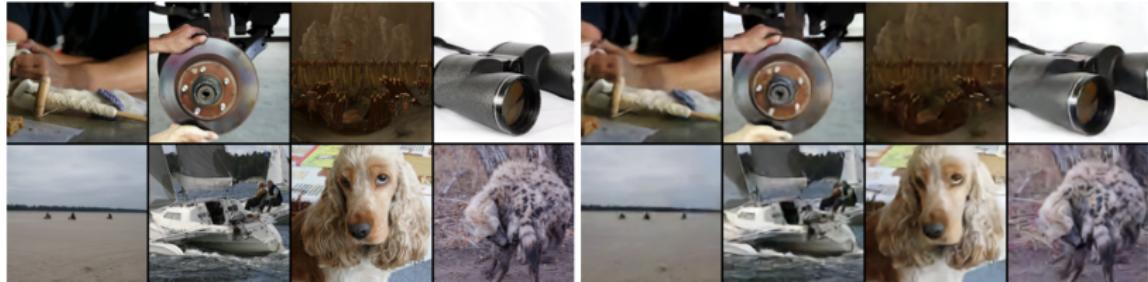
## Objective

$$\log p(x|z_q) + \|\text{sg}(z_e) - z_q\| + \beta \|z_e - \text{sg}(z_q)\|$$

- ▶ First term is ELBO part.
- ▶ Quantization operation is not differentiable.
- ▶ Straight-through gradient estimation is used to backpropagate the quantization operation.

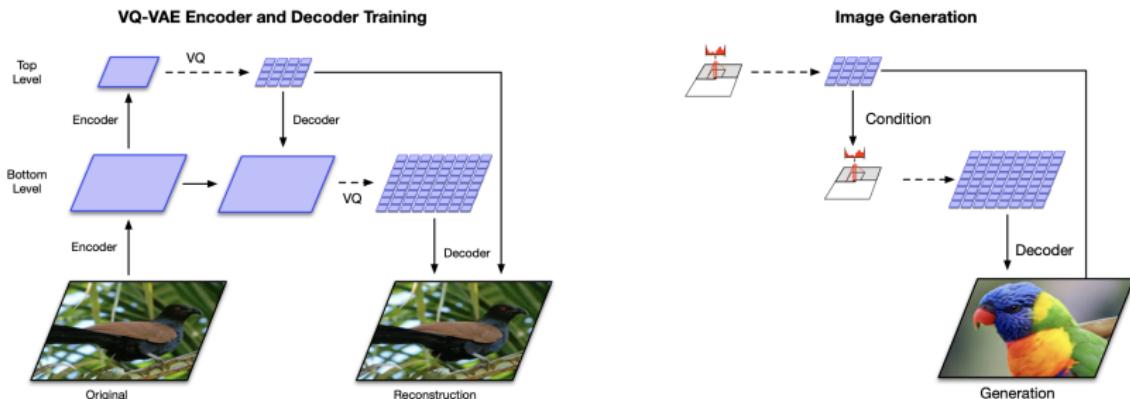
## Vector Quantized VAE

- ▶ 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  $\hat{z}$ .



# 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

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

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

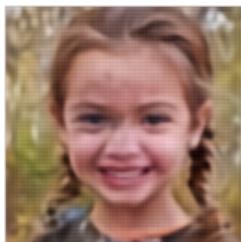
- 1:  $\mathbf{h}_{top} \leftarrow E_{top}(\mathbf{x})$   
    ▷ quantize with top codebook eq 1
- 2:  $\mathbf{e}_{top} \leftarrow Quantize(\mathbf{h}_{top})$
- 3:  $\mathbf{h}_{bottom} \leftarrow E_{bottom}(\mathbf{x}, \mathbf{e}_{top})$   
    ▷ quantize with bottom codebook eq 1
- 4:  $\mathbf{e}_{bottom}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

## 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

# Vector Quantized VAE-2

Samples 1024x1024



Samples diversity



VQ-VAE (Proposed)

BigGAN deep

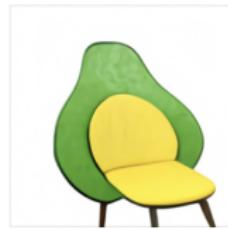
Razavi A., Oord A., Vinyals O. Generating Diverse High-Fidelity Images with VQ-VAE-2, 2019

# DALL-E

TEXT PROMPT

an armchair in the shape of an avocado [...]

AI-GENERATED IMAGES



# Summary

