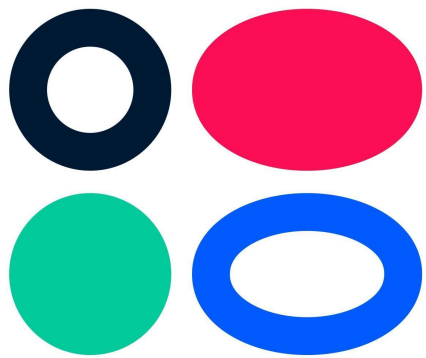
Deep Generative Models
Lecture 13

Roman Isachenko



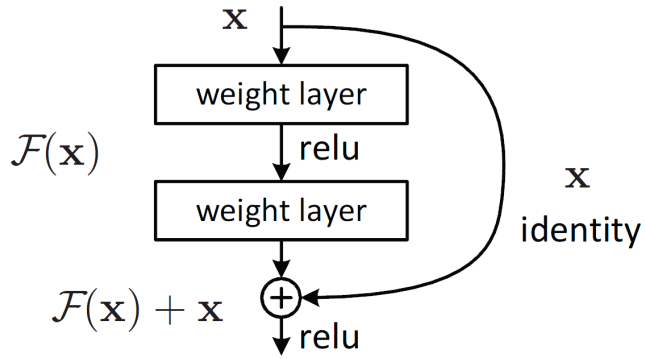
Ozon Masters

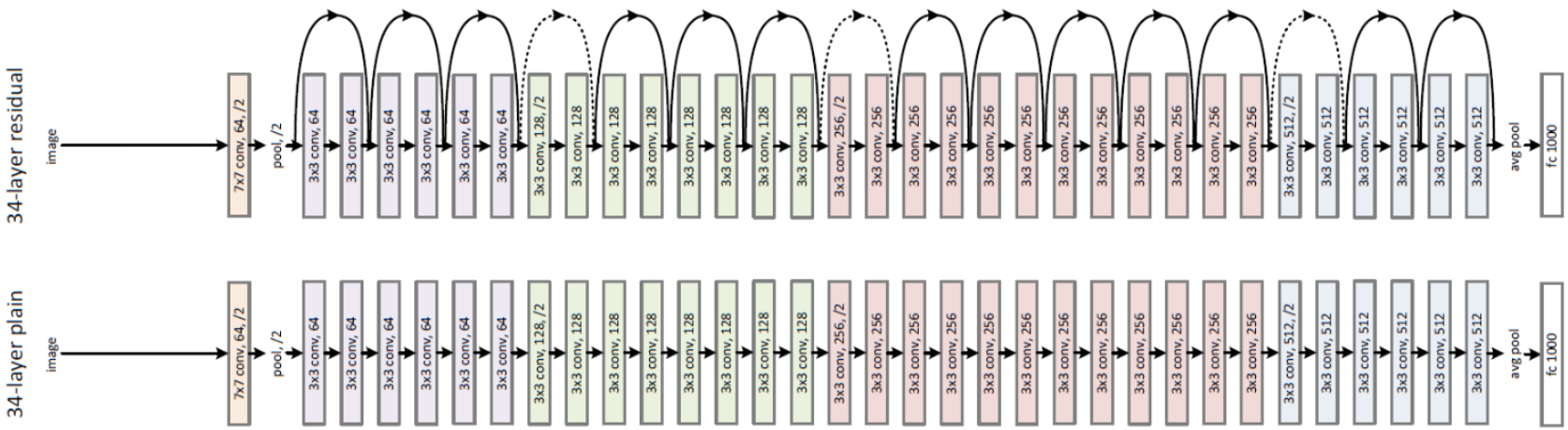
Spring, 2021

Neural ODE

- Neural networks for classification task have hundreds of layers.
- Skip connections eliminate exploding/vanishing gradients.

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





Chen R. T. Q. et al. Neural Ordinary Differential Equations, 2018

Neural ODE

Consider Ordinary Differential Equation

$$\frac{d\mathbf{z}(t)}{dt} = f(\mathbf{z}(t), \boldsymbol{\theta}); \quad \text{with initial condition } \mathbf{z}(t_0) = \mathbf{z}_0.$$

$$\mathbf{z}(t_1) = \int_{t_0}^{t_1} f(\mathbf{z}(t), \boldsymbol{\theta}) dt + \mathbf{z}_0 = \text{ODESolve}(\mathbf{z}(t_0), f, t_0, t_1, \boldsymbol{\theta}).$$

Euler update step

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

Residual block

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

- Residual learning is equavalent to Euler update step for solving ODE with $\Delta t = 1$!
- Euler update step is unstable and trivial. There are much more sophisticated methods.

Chen R. T. Q. et al. Neural Ordinary Differential Equations, 2018

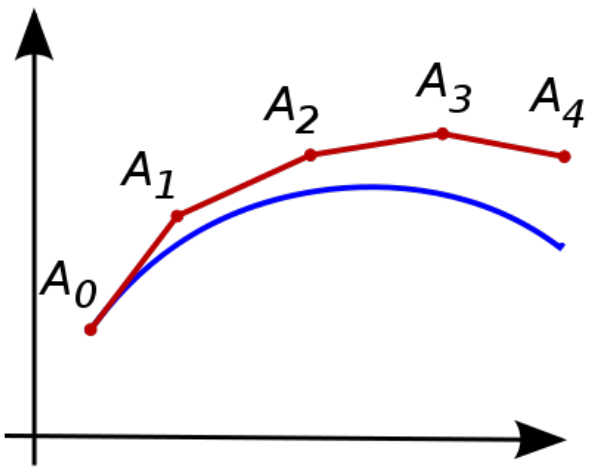
Neural ODE

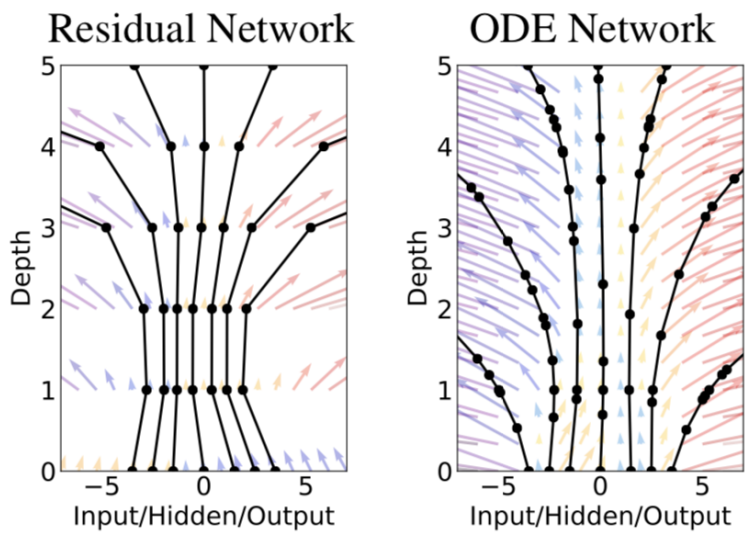
Residual block

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

- What happens as we add more layers and take smaller steps?
- In the limit, we parameterize the continuous dynamics of hidden units using an ODE specified by a neural network:

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





Chen R. T. Q. et al. Neural Ordinary Differential Equations, 2018

Neural ODE

Forward pass (loss function)

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

Note: ODESolve could be any method (not neccessary Euler).

Backward pass (gradients computation)

For fitting parameters we need gradients:

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

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

Chen R. T. Q. et al. Neural Ordinary Differential Equations, 2018

Neural ODE

Loss function (forward pass)

$$L(\mathbf{y}) = L(\mathbf{z}(t_1)) = L\left(\text{ODESolve}(\mathbf{z}(t_0), f, t_0, t_1, \boldsymbol{\theta})\right)$$

Adjoint functions

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

Theorem (Pontryagin)

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

Do we know any initilal condition?

Chen R. T. Q. et al. Neural Ordinary Differential Equations, 2018

Neural ODE

Theorem (Pontryagin)

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

Solution for adjoint function

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

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

$$\mathbf{z}(t_0) = \int_{t_1}^{t_0} f(\mathbf{z}(t), \boldsymbol{\theta}) dt + \mathbf{z}_1.$$

Chen R. T. Q. et al. Neural Ordinary Differential Equations, 2018

Neural ODE

Forward pass

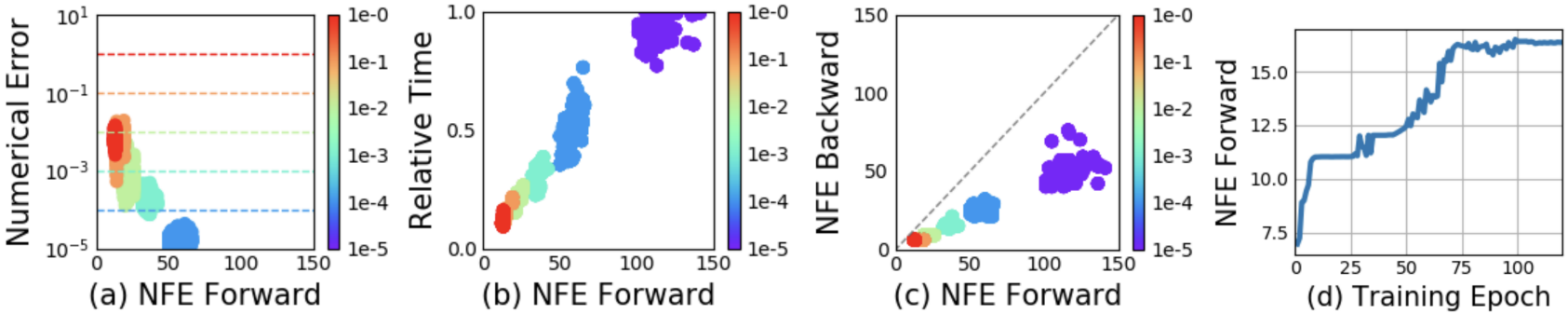
$$\mathbf{z}(t_1) = \int_{t_0}^{t_1} f(\mathbf{z}(t), \boldsymbol{\theta}) dt + \mathbf{z}_0 \quad \Rightarrow \quad \text{ODE Solver}$$

Backward pass

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

Chen R. T. Q. et al. Neural Ordinary Differential Equations, 2018

Neural ODE



Benefits

- memory efficient (there is no need to store activations);
- adaptive computation (depth is not defined explicitly);
- parameter efficient (there is only parameters of function $f(\mathbf{z}(t), \theta)$);
- scalable and invertible normalizing flows (we will discuss it today).

Chen R. T. Q. et al. Neural Ordinary Differential Equations, 2018

Continuous Normaling Flows

Discrete Normalizing Fflows

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

Planar flows

$$\mathbf{z}_{t+1} = g(\mathbf{z}_t, \theta) = \mathbf{z}_t + \mathbf{u} h(\mathbf{w}^T \mathbf{z}_t + b) = \mathbf{z}_t + f(\mathbf{z}_t, \theta).$$

Exactly residual learning.

Let consider continuous-in-time dynamic transformation of $\mathbf{z}_t$

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

Continuous dynamic for planar flows

$$\frac{d\mathbf{z}(t)}{dt} = \mathbf{u} h(\mathbf{w}^T \mathbf{z}_t + b); \quad \frac{\partial \log p(\mathbf{z}(t))}{\partial t} = -\mathbf{u}^T \frac{\partial h}{\partial \mathbf{z}(t)}.$$

Chen R. T. Q. et al. Neural Ordinary Differential Equations, 2018

Continuous Normaling Flows

Theorem

Consider the continuous dynamic $\frac{d\mathbf{z}(t)}{dt} = f(\mathbf{z}(t), \boldsymbol{\theta})$. if function f is uniformly Lipschitz continuous in $\mathbf{z}$ and continuous in t, then the change in log probability follows a differential equation

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

Continuity of function f guarantees that the solution of ODE exists and unique (Piccard theorem).

- Unlike standard finite flows, the differential equation f does not need to be bijective, since if uniqueness is satisfied, then the entire transformation is automatically bijective.
- trace$(\cdot)$ is a linear op instead of det$(\cdot)$

$$\frac{d\mathbf{z}(t)}{dt} = \sum_{j=1}^{M} f_j(\mathbf{z}(t), \boldsymbol{\theta}); \quad \frac{\partial \log p(\mathbf{z}(t))}{\partial t} = -\sum_{j=1}^{M} \text{trace}\left(\frac{\partial f_j}{\partial \mathbf{z}(t)}\right).$$

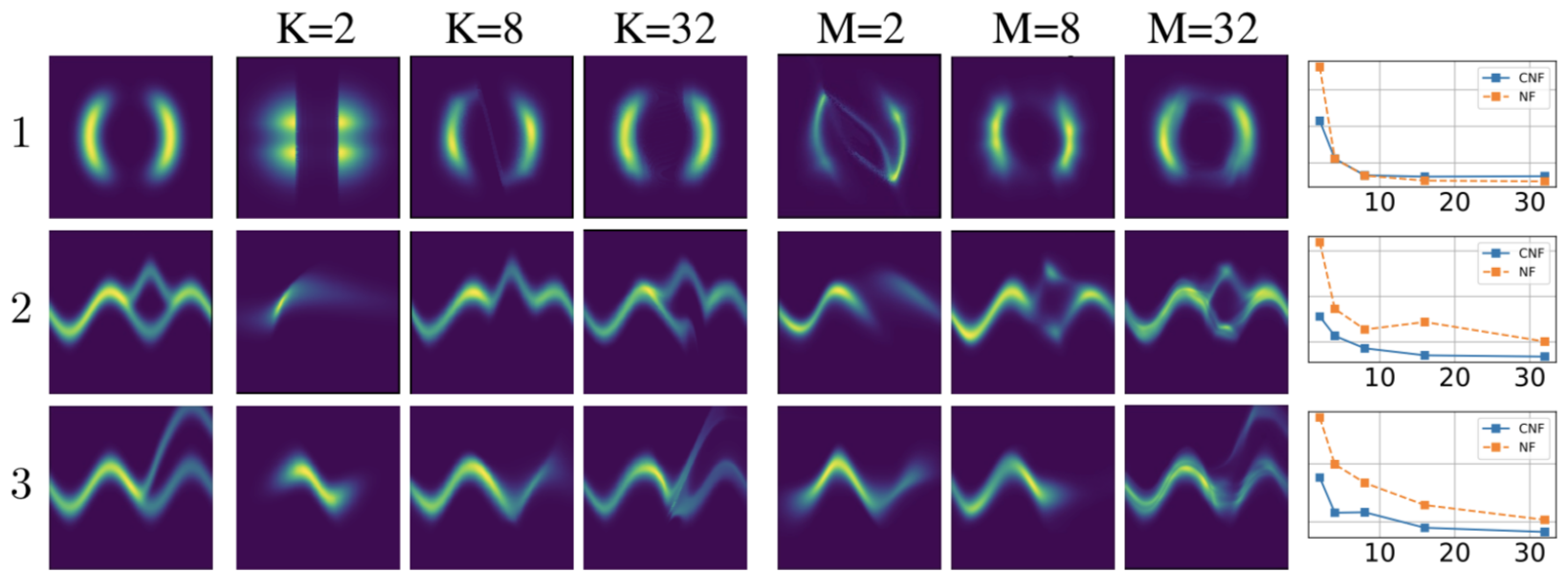
Chen R. T. Q. et al. Neural Ordinary Differential Equations, 2018

Continuous NF

Solution for continuous NF

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

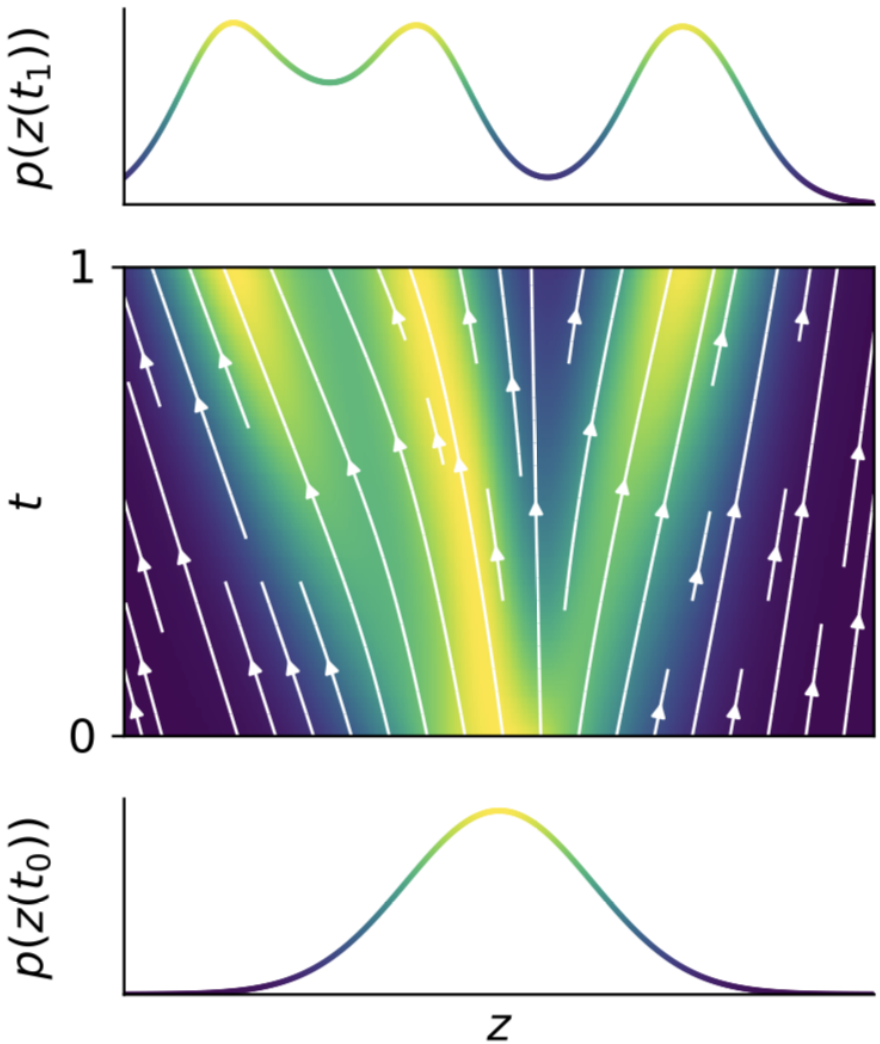
$$\log p(\mathbf{z}(t_1)) = \log p(\mathbf{z}(t_0)) - \int_{t_0}^{t_1} \text{trace}\left(\frac{\partial f}{\partial \mathbf{z}(t)}\right) dt.$$



Chen R. T. Q. et al. Neural Ordinary Differential Equations, 2018

Continuous NF

- Standard normalizing flows need invertible f.
- In general, it costs $O(d^3)$ to get det of Jacobian.
- Continuous flows need smooth f.
- In general, it costs $O(d^2)$ to get trace of Jacobian.



Chen R. T. Q. et al. Neural Ordinary Differential Equations, 2018

FFJORD

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

Hutchinson's trace estimator

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

Unbiased estimation

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

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

FFJORD

Comparison of generative modelling approaches

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

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

FFJORD

Density estimation

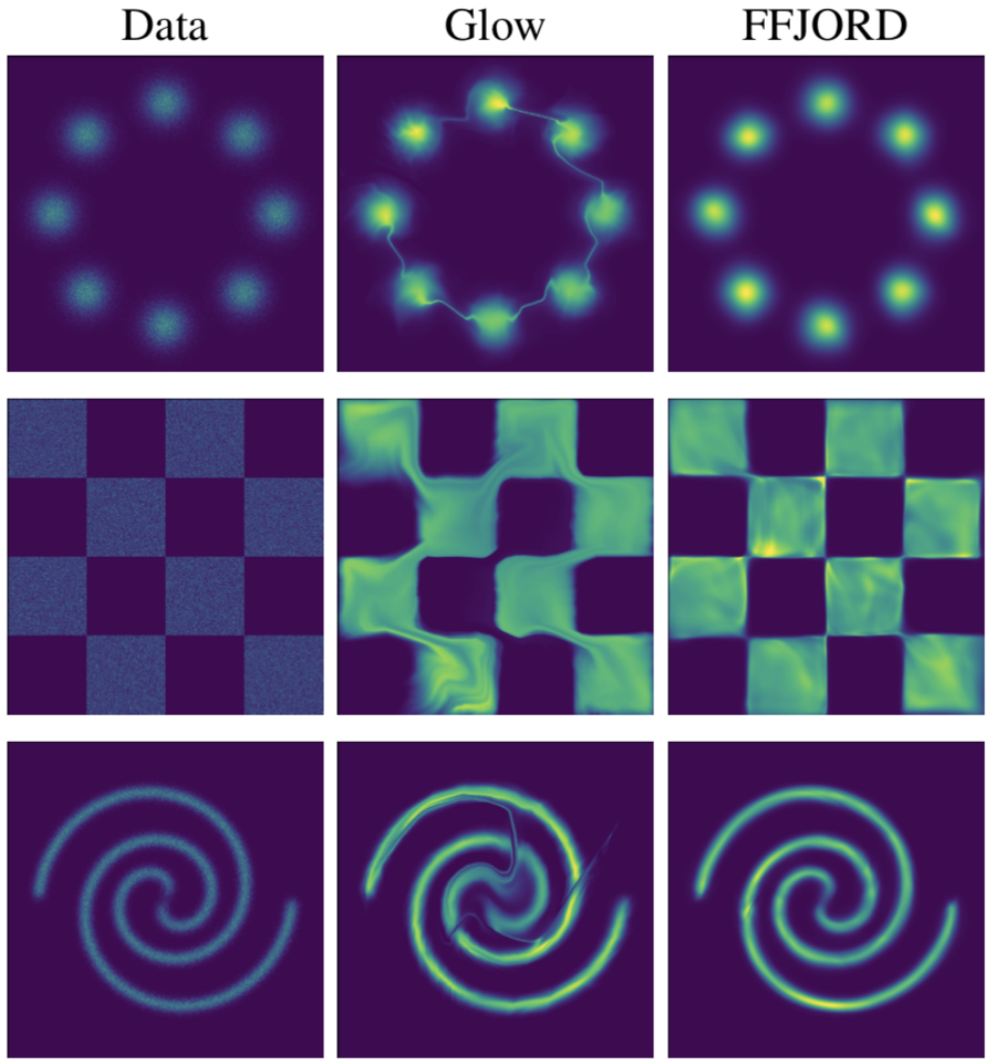
	POWER	GAS	HEPMASS	MINIBOONE	BSDS300	MNIST	CIFAR10
Real NVP	-0.17	-8.33	18.71	13.55	-153.28	1.06*	3.49*
Glow	-0.17	-8.15	18.92	11.35	-155.07	1.05*	**3.35***
FFJORD	**-0.46**	**-8.59**	**14.92**	**10.43**	**-157.40**	**0.99*** (1.05†)	3.40*
MADE	3.08	-3.56	20.98	15.59	-148.85	2.04	5.67
MAF	-0.24	-10.08	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

	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	$\mathbf{82.82 \pm .01}$	$\mathbf{98.33 \pm .09}$	$\mathbf{4.39 \pm .01}$	$\mathbf{104.03 \pm .43}$

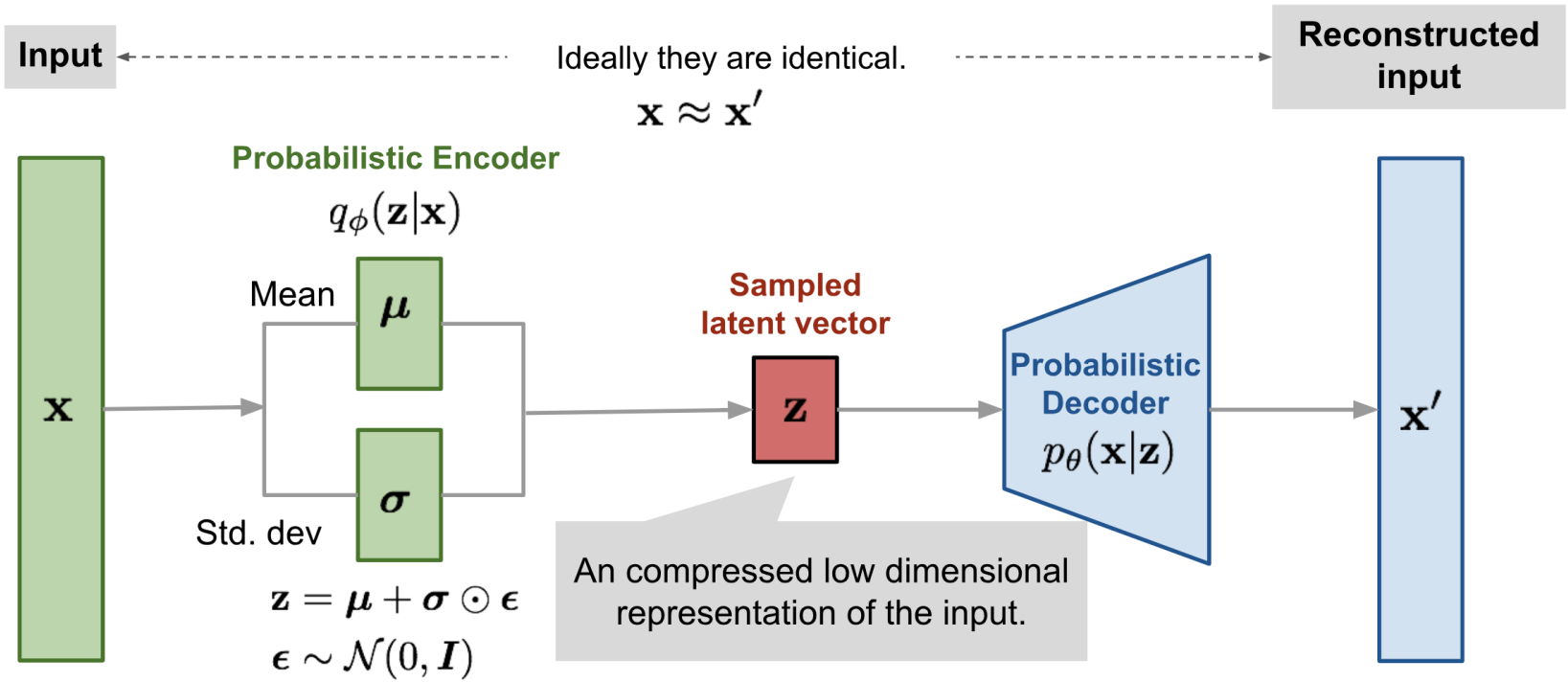
Grathwohl W. et al. FFJORD: Free-form Continuous Dynamics for Scalable Reversible Generative Models, 2018

FFJORD



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

Discrete VAE



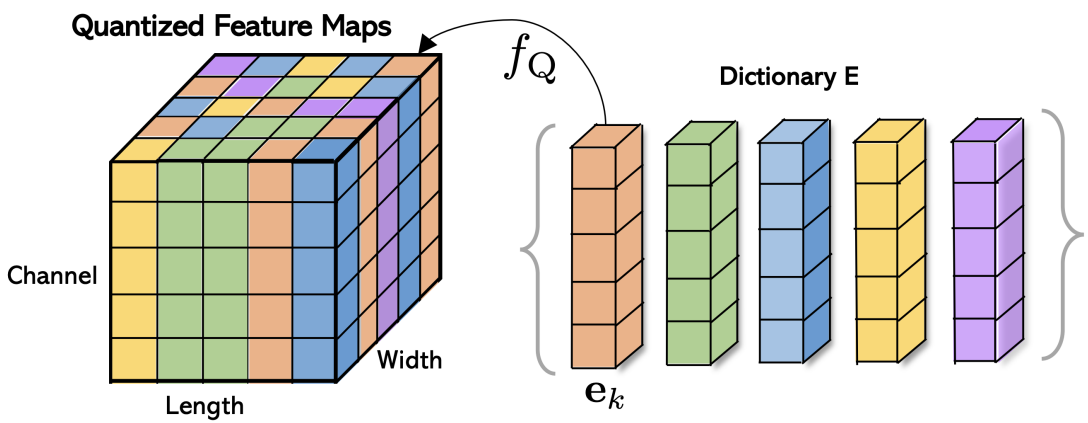
- Previous VAE models had **continuous** latent variables $\mathbf{z}$.
- **Discrete** representations $\mathbf{z}$ are potentially a more natural fit for many of the modalities.
- Powerful autoregressive models (like PixelCNN) have been developed for modelling distributions over discrete variables.

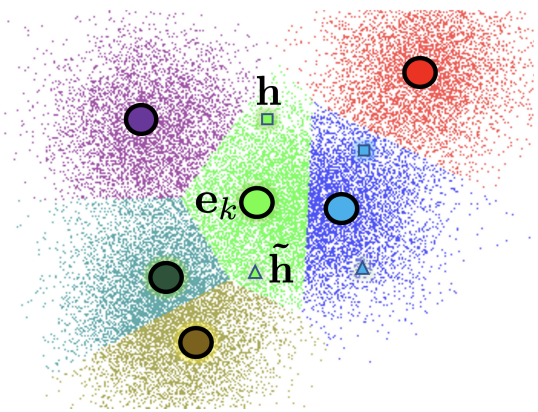
Vector Quantized VAE

- 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 $\mathbf{z} = \mathrm{NN}_e(\mathbf{x}) \in \mathbb{R}^{W \times H \times C}$ 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





Zhao Y. et al. Feature Quantization Improves GAN Training, 2020

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

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

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

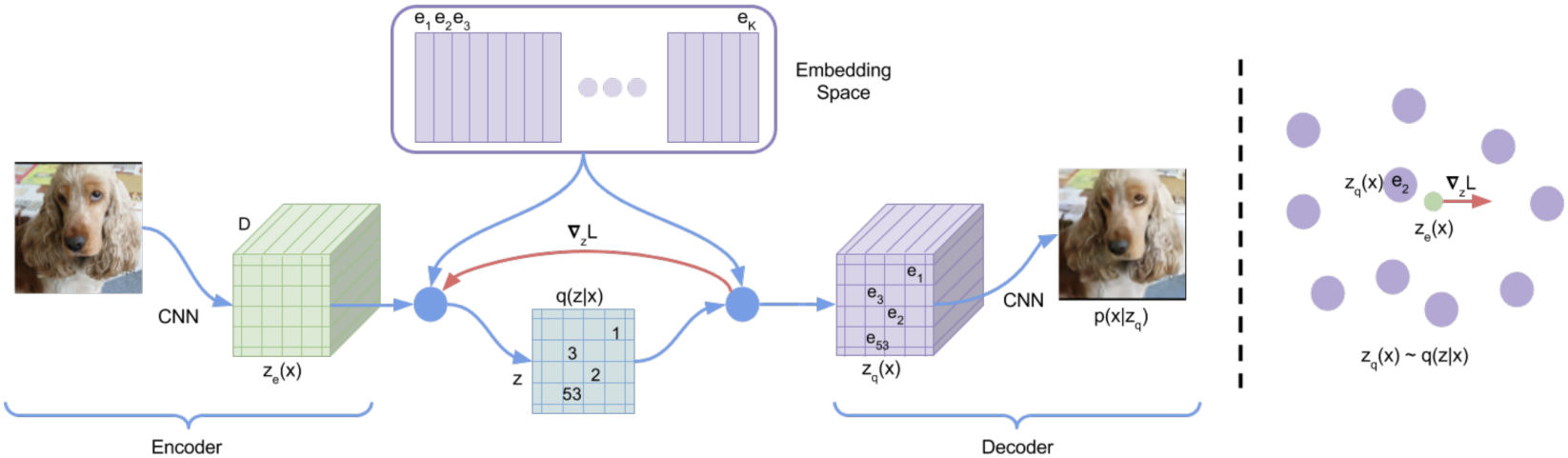
ELBO objective

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

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

Oord A., Vinyals O., Kavukcuoglu K. Neural Discrete Representation Learning, 2017

Vector Quantized VAE



Objective

$$\log p(\mathbf{x}|\mathbf{z}_q) + \|\text{sg}(\mathbf{z}_e) - \mathbf{z}_q\| + \beta\|\mathbf{z}_e - \text{sg}(\mathbf{z}_q)\|$$

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

Oord A., Vinyals O., Kavukcuoglu K. Neural Discrete Representation Learning, 2017

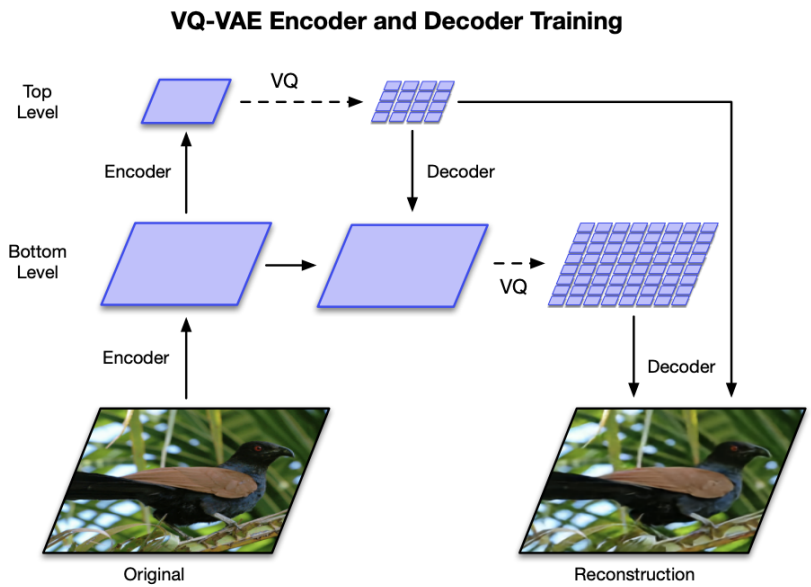
Vector Quantized VAE

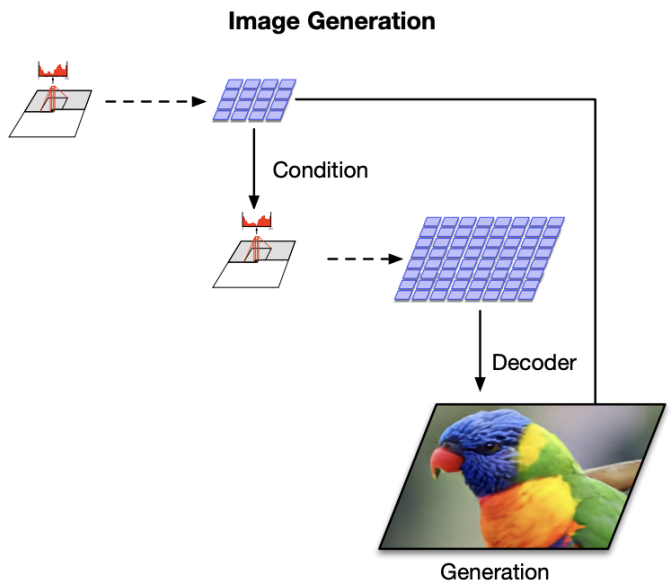
- The prior distribution over the discrete latents $p(\hat{\mathbf{z}})$ is a categorical distribution.
- It could be made autoregressive by depending on other $\hat{\mathbf{z}}$ in the feature map.
- While training the VQ-VAE, the prior is kept constant and uniform.
- After training, fit an autoregressive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

Oord A., Vinyals O., Kavukcuoglu K. Neural Discrete Representation Learning, 2017

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.





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

Vector Quantized VAE-2

Algorithm 1 VQ-VAE training (stage 1)

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

$\mathbf{h}_{top} \leftarrow E_{top}(\mathbf{x})$

▷ quantize with top codebook eq 1

$\mathbf{e}_{top} \leftarrow Quantize(\mathbf{h}_{top})$

$\mathbf{h}_{bottom} \leftarrow E_{bottom}(\mathbf{x}, \mathbf{e}_{top})$

▷ quantize with bottom codebook eq 1

$\mathbf{e}_{bottom} \leftarrow Quantize(\mathbf{h}_{bottom})$

$\hat{\mathbf{x}} \leftarrow D(\mathbf{e}_{top}, \mathbf{e}_{bottom})$

▷ Loss according to eq 2

$\theta \leftarrow Update(\mathcal{L}(\mathbf{x}, \hat{\mathbf{x}}))$

Algorithm 2 Prior training (stage 2)

$\mathbf{T}_{top}, \mathbf{T}_{bottom} \leftarrow \emptyset$ ▷ training set

for $\mathbf{x} \in$ training set **do**

  $\mathbf{e}_{top} \leftarrow Quantize(E_{top}(\mathbf{x}))$

  $\mathbf{e}_{bottom} \leftarrow Quantize(E_{bottom}(\mathbf{x}, \mathbf{e}_{top}))$

  $\mathbf{T}_{top} \leftarrow \mathbf{T}_{top} \cup \mathbf{e}_{top}$

  $\mathbf{T}_{bottom} \leftarrow \mathbf{T}_{bottom} \cup \mathbf{e}_{bottom}$

end for

$p_{top} = \texttt{TrainPixelCNN}(\mathbf{T}_{top})$

$p_{bottom} = \texttt{TrainCondPixelCNN}(\mathbf{T}_{bottom}, \mathbf{T}_{top})$

▷ Sampling procedure

while true **do**

  $\mathbf{e}_{top} \sim p_{top}$

  $\mathbf{e}_{bottom} \sim p_{bottom}(\mathbf{e}_{top})$

  $\mathbf{x} \leftarrow D(\mathbf{e}_{top}, \mathbf{e}_{bottom})$

end while

h_{top} $h_{\text{top}}, h_{\text{middle}}$ $h_{\text{top}}, h_{\text{middle}}, h_{\text{bottom}}$ Original

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

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

Summary