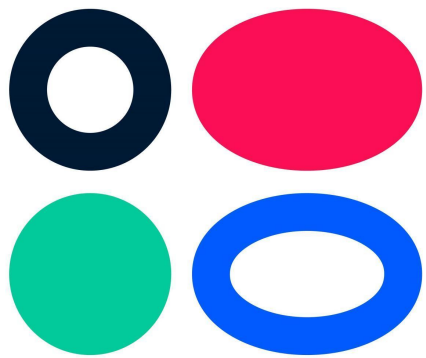
Deep Generative Models
Lecture 12

Roman Isachenko



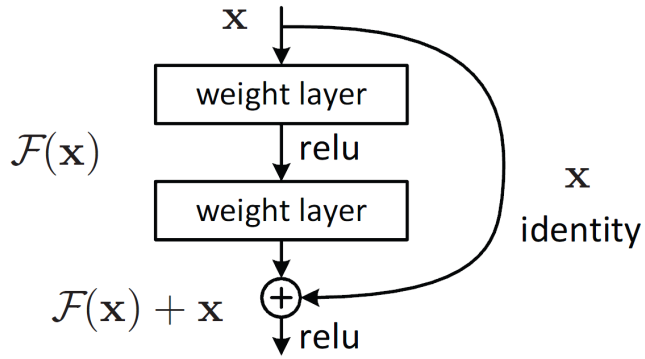
Ozon Masters

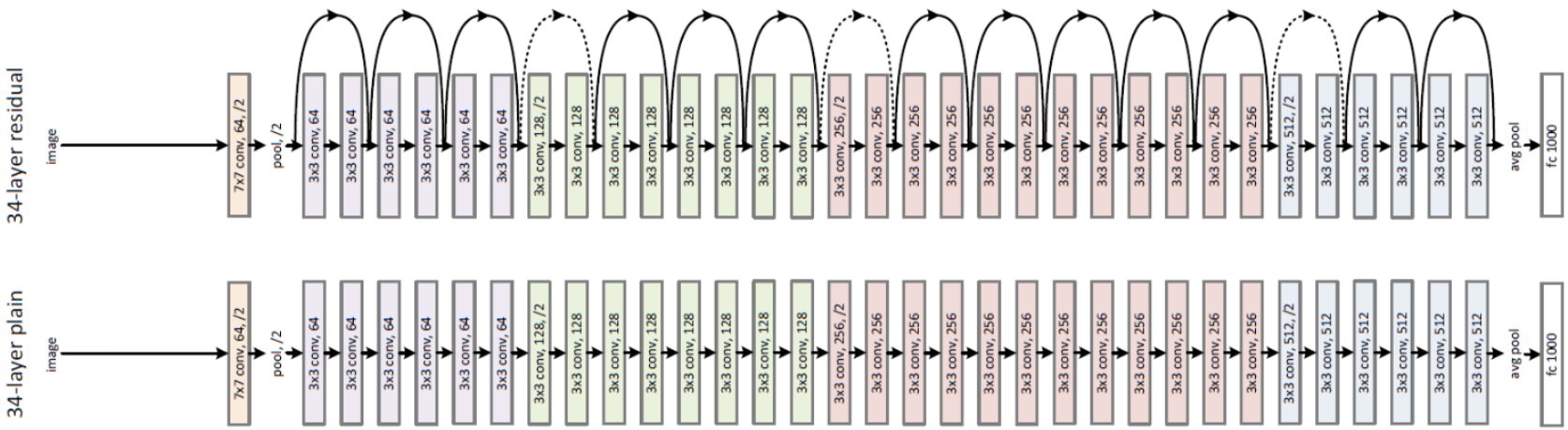
Spring, 2021

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

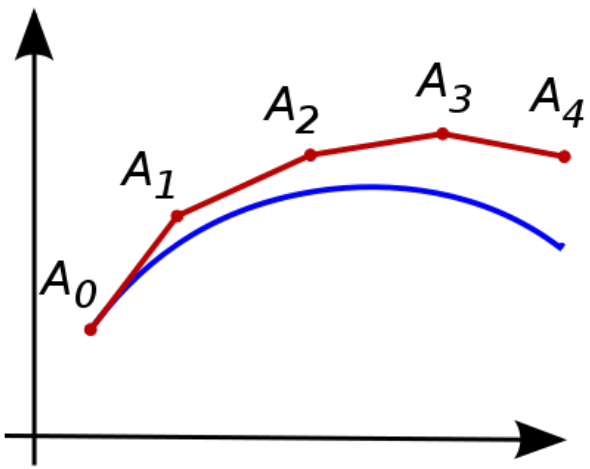
Neural ODE

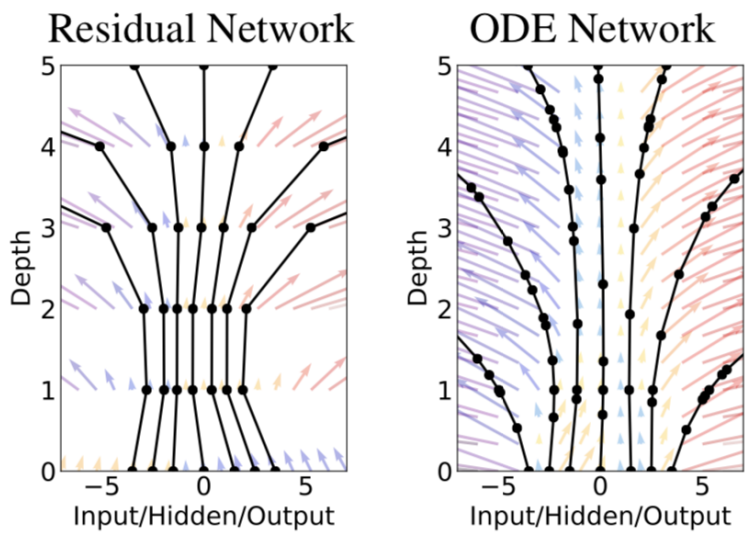
Residual block

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

- 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 $\boldsymbol{\theta}$.

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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?

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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

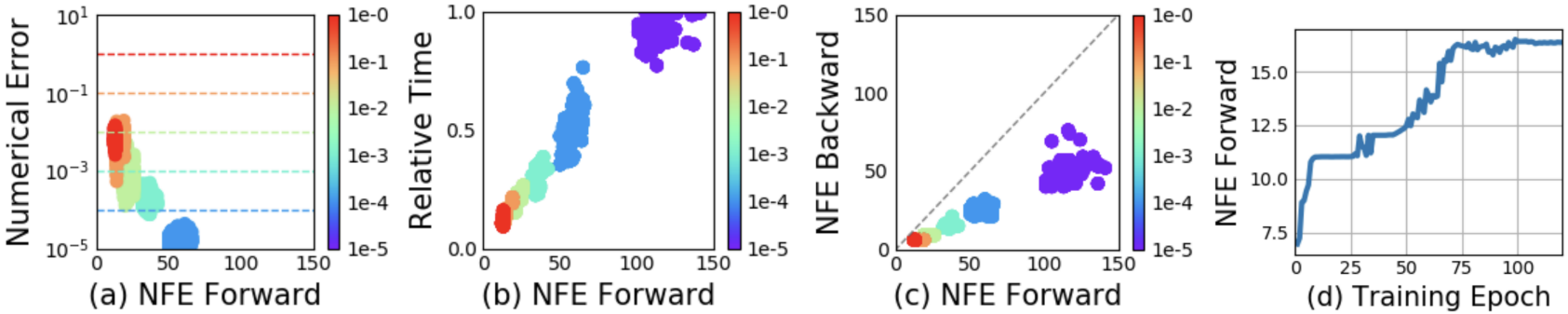
$$\mathbf{z}(t_1) = \int_{t_0}^{t_1} f(\mathbf{z}(t), \boldsymbol{\theta}) dt + \mathbf{z}_0 \quad \Rightarrow \quad \text{ODE Solver}$$

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$(\cdot)$

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

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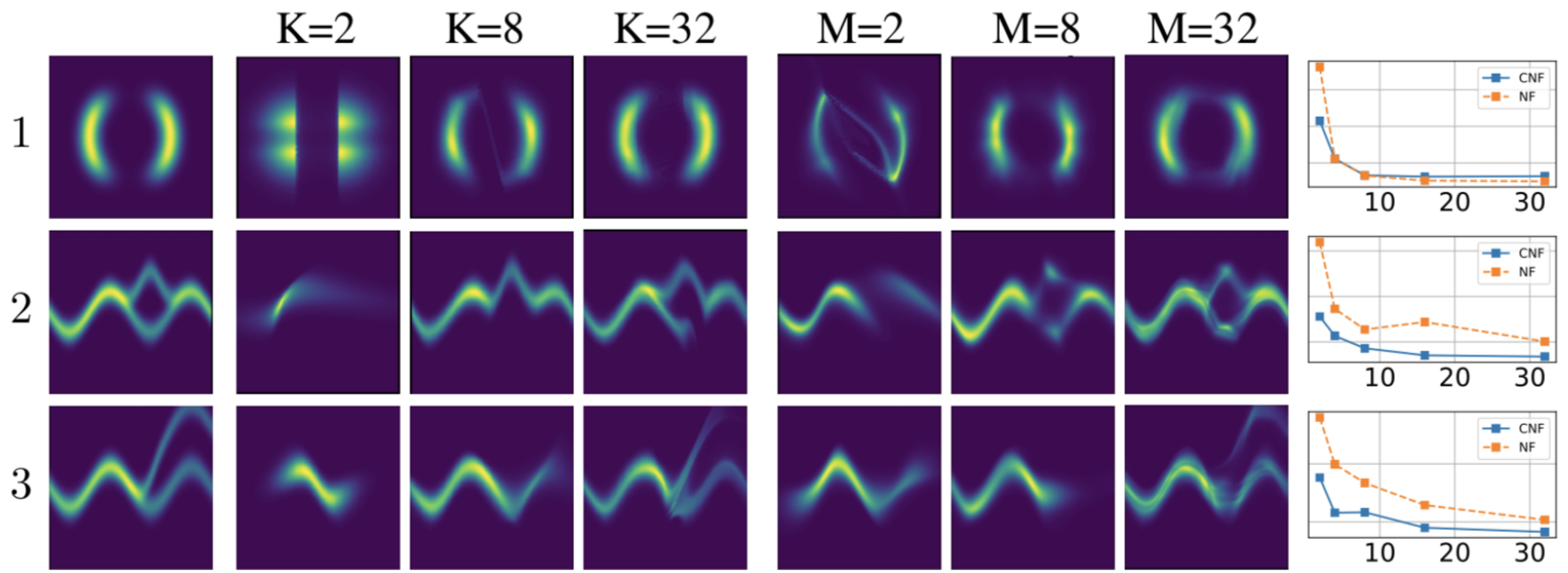
Continuous NF

Solution for continuous NF

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

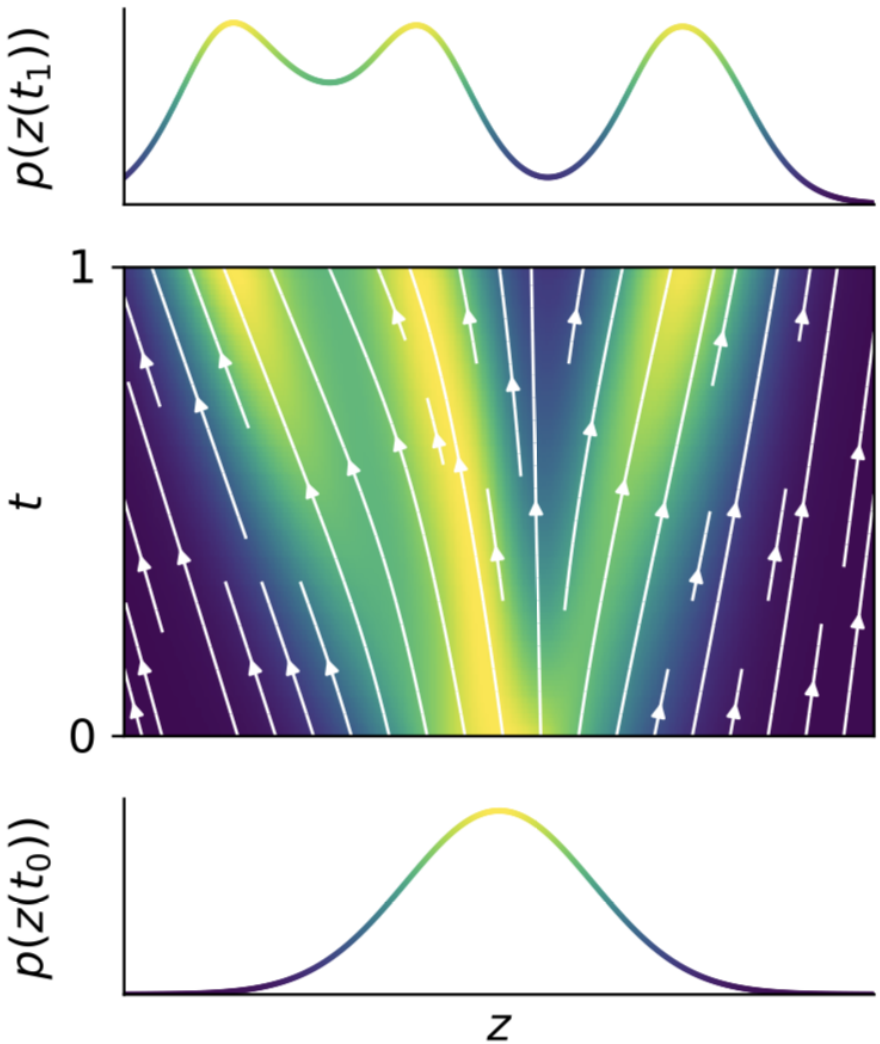
$$\log p(\mathbf{z}(t_1)) = \log p(\mathbf{z}(t_0)) - \int_{t_0}^{t_1} \text{trace}\left(\frac{\partial f}{\partial \mathbf{z}(t)}\right) dt.$$



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

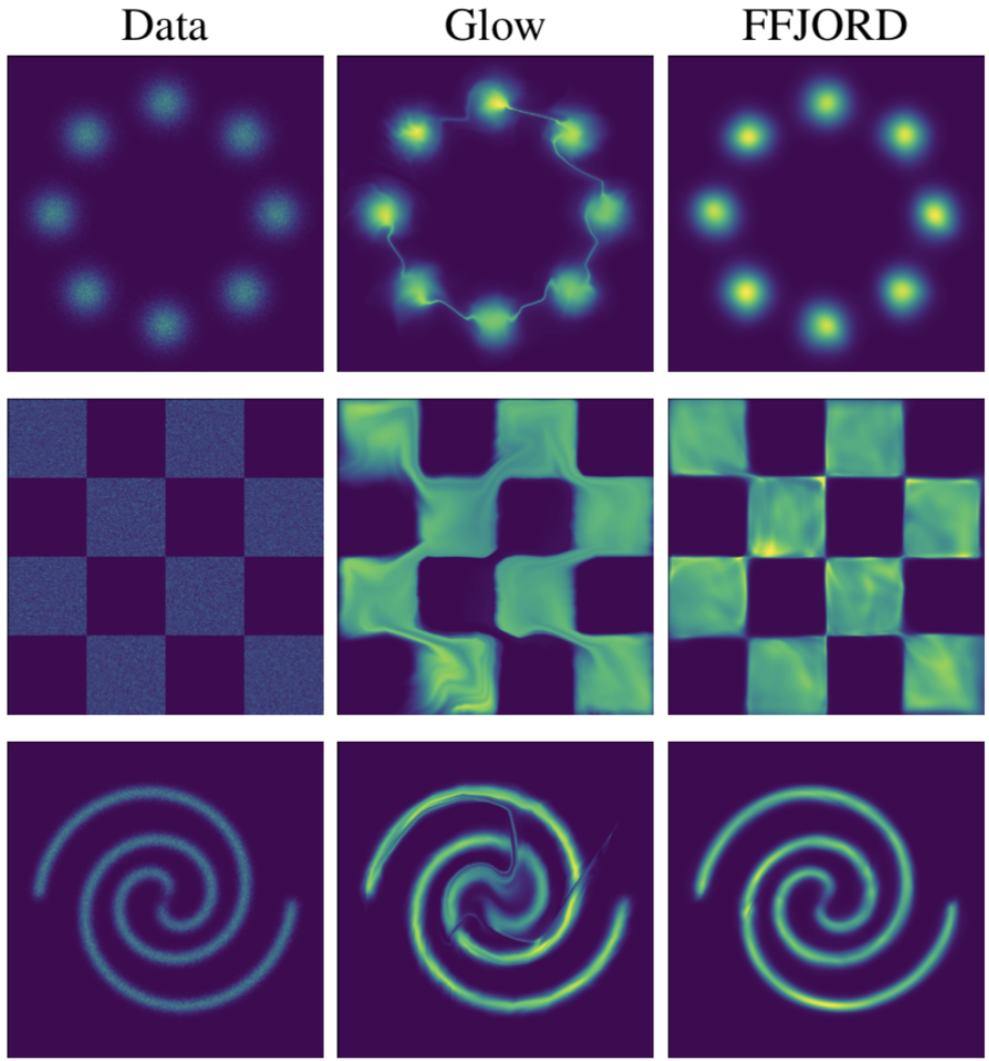
	POWER	GAS	HEPMASS	MINIBOONE	BSDS300	MNIST	CIFAR10
Real NVP	-0.17	-8.33	18.71	13.55	-153.28	1.06*	3.49*
Glow	-0.17	-8.15	18.92	11.35	-155.07	1.05*	**3.35***
FFJORD	**-0.46**	**-8.59**	**14.92**	**10.43**	**-157.40**	**0.99*** (1.05†)	3.40*
MADE	3.08	-3.56	20.98	15.59	-148.85	2.04	5.67
MAF	-0.24	-10.08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

- Before we have discussed VAE with **continuous** latent variables.
- VAE suffers from posterior collapse if the decoder too powerful (PixelVAE, VLAE tries to solve this problem).
- **Discrete** representations are potentially a more natural fit for many of the modalities.
- Powerful autoregressive models (like PixelCNNN) have been developed for modelling distributions over discrete variables.
- However, to construct the model with discrete representations is not so easy (e.g. variance of such estimators is a problem).

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

Vector Quantized VAE

- Latent embedding space $\{\mathbf{e}_j\}_{j=1}^{K}$, where $\mathbf{e}_j \in \mathbb{R}^D$, K is the size of a discrete latent space.
- $\mathbf{z}_e(\mathbf{x})$ is an encoder output.
- z is a discrete random variable calculated by a nearest neighbour look-up using the shared embedding space. The posterior categorical distribution is defined as

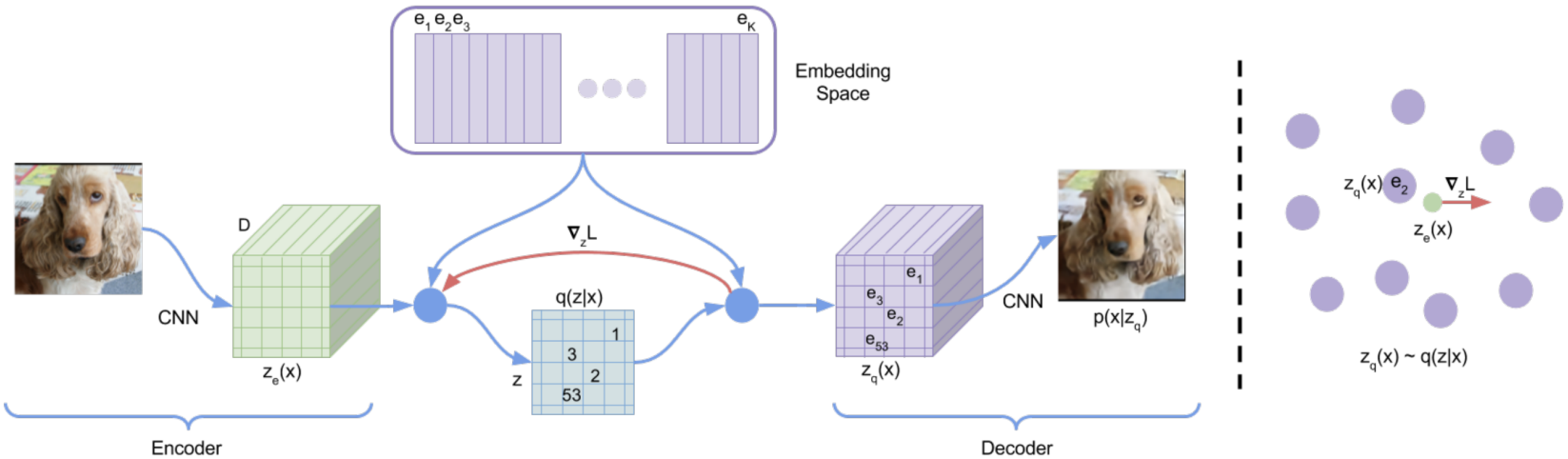
$$q(z = k|\mathbf{x}) = \begin{cases} 1, & \text{for } k = \arg\min_j \|\mathbf{z}_e(\mathbf{x}) - \mathbf{e}_j\| \\ 0, & \text{otherwise.} \end{cases}$$

- VAE proposal distribution $q(z|\mathbf{x})$ is deterministic. If prior $p(z)$ is a uniform then $KL(q(z|\mathbf{x})||p(z))$ term in ELBO is constant (equals to $\log K$).
- Quantized representation is defined as follows

$$\mathbf{z}_q(\mathbf{x}) = \mathbf{e}_k, \quad \text{where } k = \arg\min_j \|\mathbf{z}_e(\mathbf{x}) - \mathbf{e}_j\|$$

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

Vector Quantized VAE



Objective

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

- 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

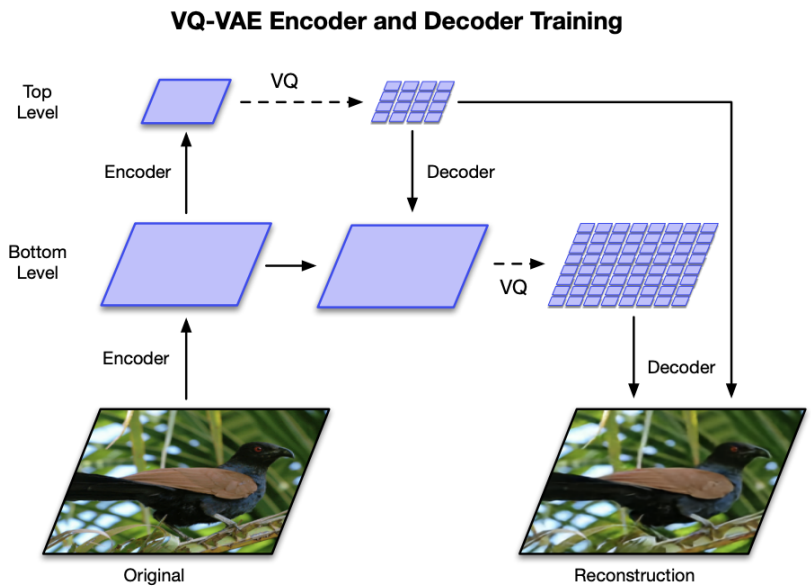
Vector Quantized VAE

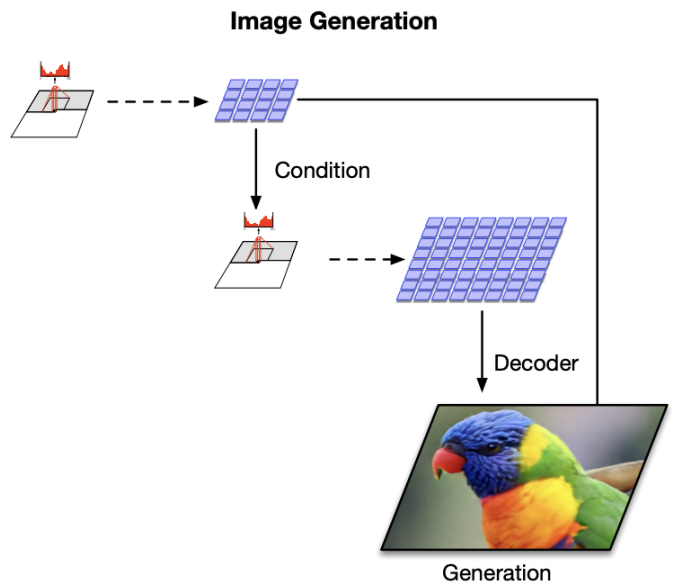
- The prior distribution over the discrete latents $p(\mathbf{z})$ is a categorical distribution.
- It could be made autoregressive by depending on other $\mathbf{z}$ in the feature map.
- Whilst training the VQ-VAE, the prior is kept constant and uniform.
- After training, fit an autoregressive distribution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

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.





https://arxiv.org/abs/1906.00446

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

FFHQ 1024x1024

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

Vector Quantized VAE-2

VQ-VAE (Proposed) **BigGAN deep**

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

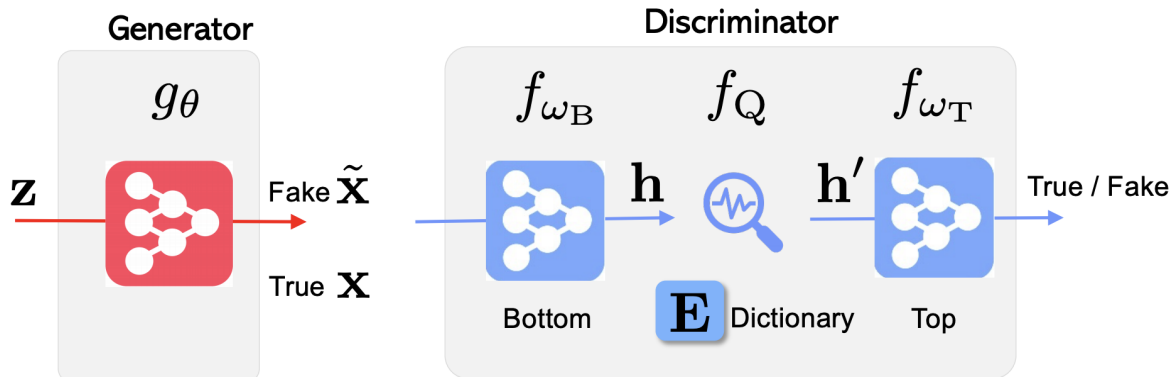
Feature Quantized GAN

- 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

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

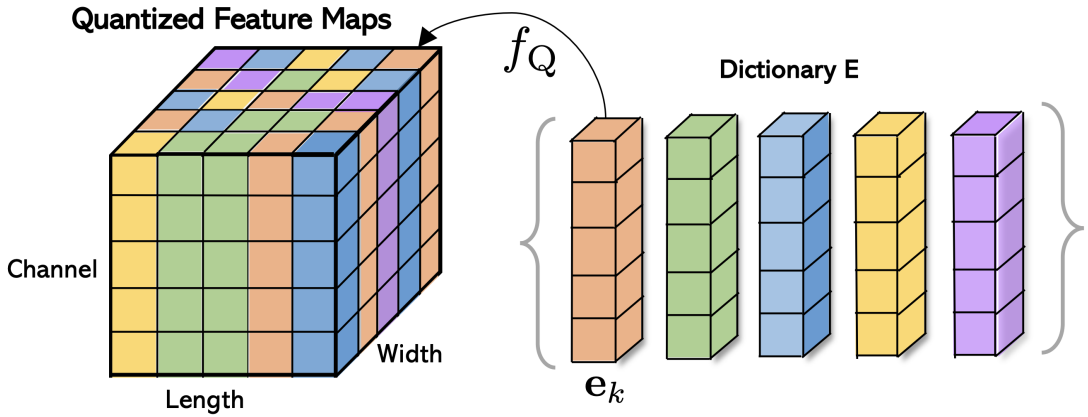
Here f_Q is a vector quantization operation.

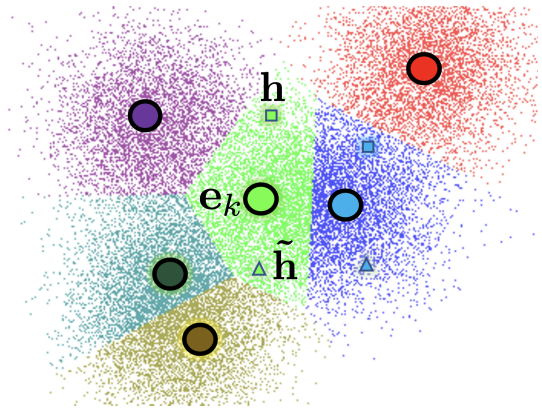


Zhao Y. et al. Feature Quantization Improves GAN Training, 2020

Feature Quantized GAN

Quantization procedure





Quantized features

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

Feature Quantized GAN

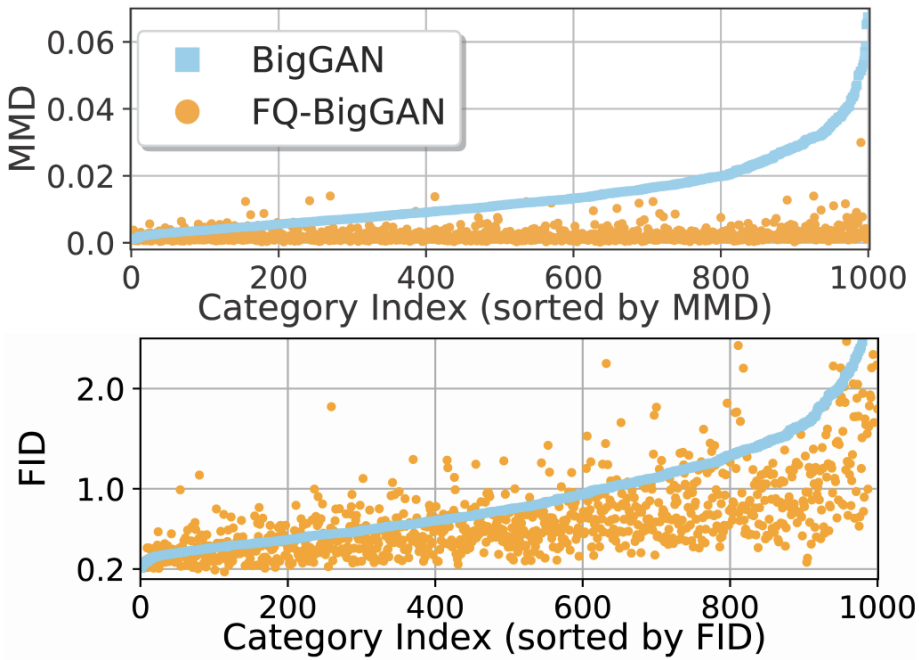
ImageNet-1000

Models		64 × 64	128 × 128
		FID* ↓ / IS* ↑	FID* ↓ / IS* ↑
Half	TAC-GAN	-	23.75 / 28.86±0.29‡
	BigGAN	12.75 / 21.84±0.34	22.77 / 38.05±0.79‡
	FQ-BigGAN	**12.62 / 21.99**±0.32	**19.11 / 41.92**±1.15
256K	BigGAN	10.55 / 25.43±0.15	14.88 / 63.03±1.42†
	FQ-BigGAN	**9.67 / 25.96**±0.24	**13.77** / 54.36±1.07

FFHQ

Resolution	32^2	64^2	128^2	1024^2
StyleGAN	3.28	4.82	6.33	5.24
FQ-StyleGAN	**3.01**	**4.36**	**5.98**	**4.89**

Per class metrics for ImageNet



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

Summary