Deep Generative Models

Lecture 13

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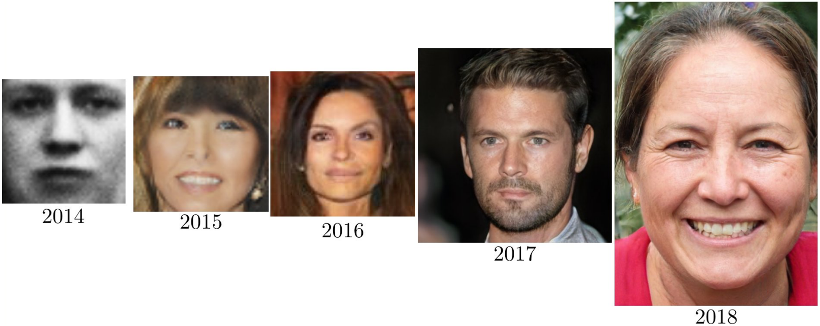
Ozon Masters

Spring, 2022

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

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

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

We have to estimate density ratio

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

Adversarial Variational Bayes

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

Mescheder L., Nowozin S., Geiger A. Adversarial variational bayes: Unifying variational autoencoders and generative adversarial networks, 2017

Outline

Neural ODE

Consider Ordinary Differential Equation

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

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

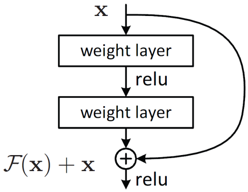
Euler update step

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

Residual block

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

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



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

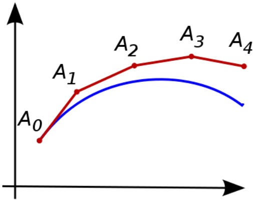
Neural ODE

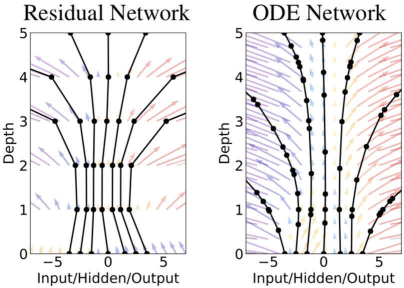
Residual block

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

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:

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





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

Neural ODE

Forward pass (loss function)

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

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

Backward pass (gradients computation)

For fitting parameters we need gradients:

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

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 $\boldsymbol{\theta}$.

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

Neural ODE

Adjoint functions

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

Theorem (Pontryagin)

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

Do we know any initilal condition?

Solution for adjoint function

$$\frac{\partial L}{\partial \boldsymbol{\theta}(t_0)} = \mathbf{a}_{\boldsymbol{\theta}}(t_0) = -\int_{t_1}^{t_0} \mathbf{a}_{\mathbf{z}}(t)^T \frac{\partial f(\mathbf{z}(t), \boldsymbol{\theta})}{\partial \boldsymbol{\theta}(t)} dt + 0$$

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

Note: These equations are solved back in time.

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

Neural ODE

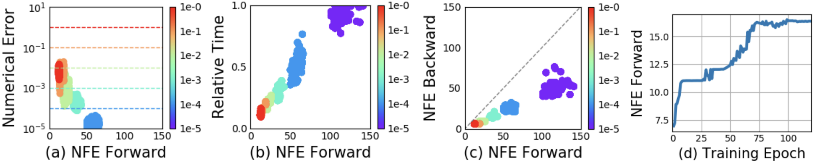
Forward pass

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

Backward pass

$$\left.\begin{aligned}
\frac{\partial L}{\partial \boldsymbol{\theta}(t_0)} &= \mathbf{a}_{\boldsymbol{\theta}}(t_0) = -\int_{t_1}^{t_0} \mathbf{a}_{\mathbf{z}}(t)^T \frac{\partial f(\mathbf{z}(t), \boldsymbol{\theta})}{\partial \boldsymbol{\theta}(t)} dt + 0 \\
\frac{\partial L}{\partial \mathbf{z}(t_0)} &= \mathbf{a}_{\mathbf{z}}(t_0) = -\int_{t_1}^{t_0} \mathbf{a}_{\mathbf{z}}(t)^T \frac{\partial f(\mathbf{z}(t), \boldsymbol{\theta})}{\partial \mathbf{z}(t)} dt + \frac{\partial L}{\partial \mathbf{z}(t_1)} \\
\mathbf{z}(t_0) &= -\int_{t_1}^{t_0} f(\mathbf{z}(t), \boldsymbol{\theta})dt + \mathbf{z}_1.
\end{aligned}\right\} \Rightarrow \text{ODE Solver}$$

Note: These scary formulas are the standard backprop in the discrete case.



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

Continuous Normalizing Flows

Discrete Normalizing Flows

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

Continuous-in-time dynamic transformation

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

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

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

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

Papamakarios G. et al. Normalizing flows for probabilistic modeling and inference, 2019

Continuous Normalizing Flows

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

Theorem (Fokker-Planck)

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

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

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

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

Adjoint method is used to integral evaluation.

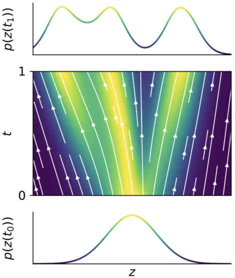
Chen R. T. Q. et al. Neural Ordinary Differential Equations, 2018

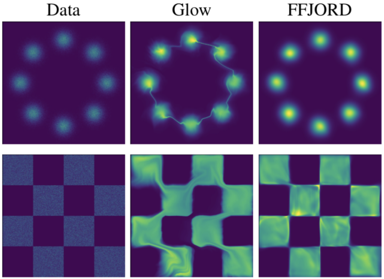
Continuous Normalizing Flows

Forward transform + log-density

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

- 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.





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

FFJORD

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

Density estimation (forward KL)

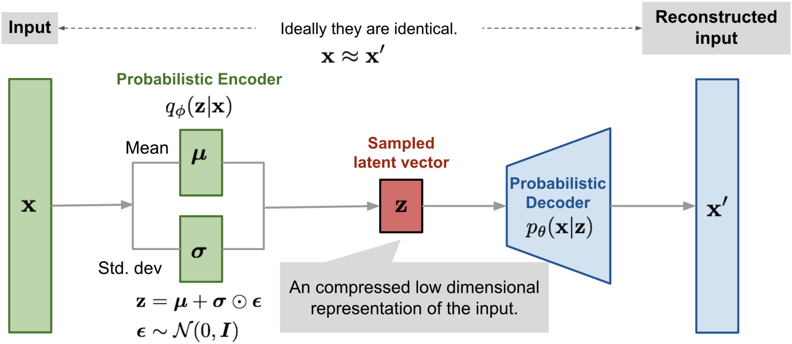
	POWER	GAS	HEPMASS	MINIBOONE	BSDS300	MNIST	CIFAR10
Real NVP	-0.17	-8.33	18.71	13.55	-153.28	1.06*	3.49*
Glow	-0.17	-8.15	18.92	11.35	-155.07	1.05*	**3.35***
FFJORD	**-0.46**	**-8.59**	**14.92**	**10.43**	**-157.40**	**0.99*** (1.05†)	3.40*

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	$83.32 \pm .06$	$99.00 \pm .04$	$4.45 \pm .04$	$104.62 \pm .29$
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

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.

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

$$z = \arg\max_k (\log \pi_k + G_k), \quad \sum_k \pi_k = 1$$

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 τ is a temperature parameter.

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

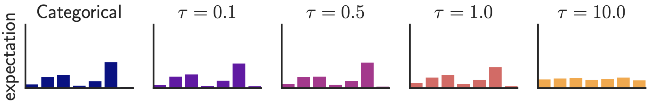
Discrete VAE

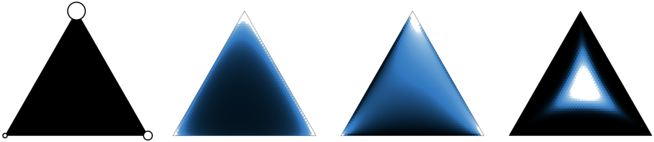
Gumbel-Softmax relaxation

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 τ is a temperature parameter. Now we have differentiable operation.





(a) $\lambda = 0$ (b) $\lambda = 1/2$ (c) $\lambda = 1$ (d) $\lambda = 2$

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

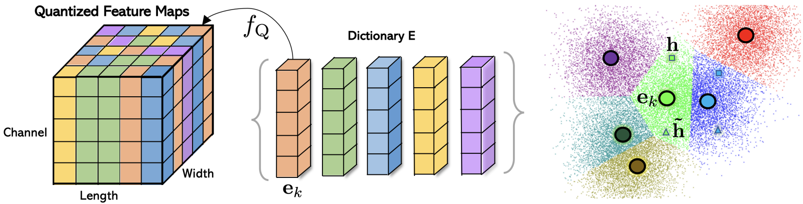
Jang E., Gu S., Poole B. Categorical reparameterization with Gumbel-Softmax, 2016

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

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

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

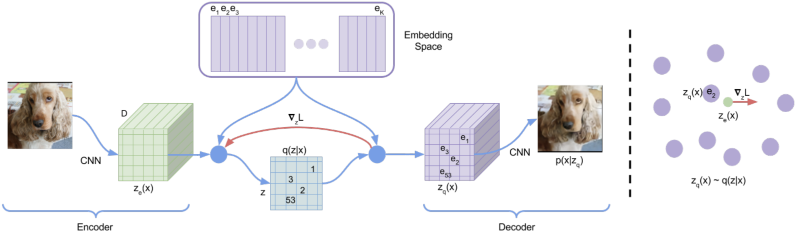
ELBO objective

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

- VAE proposal distribution $q(\hat{\mathbf{z}}|\mathbf{x})$ 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

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

- 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-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

Deterministic VQ-VAE posterior

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

- It is possible to use Gumbel-Softmax trick to relax this distribution to continuous one.
- Since latent space is discrete we could train autoregressive transformers in it.
- It is a natural way to incorporate text and image spaces.

TEXT PROMPT

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

AI-GENERATED IMAGES

Ramesh A. et al. Zero-shot text-to-image generation, 2021

Summary

- Residual networks could be interpreted as solution of ODE with Euler method.
- Adjoint method generalizes backpropagation procedure and allows to train Neural ODE solving ODE for adjoint function back in time.
- Fokker-Planck theorem allows to construct continuous-in-time normalizing flow with less functional restrictions.
- FFJORD model makes such kind of flows scalable.
- Gumbel-Softmax and Quantization are the two ways to create VAE with discrete latent space.
- It becomes more and more popular to use discrete latent spaces in the fields of image/video/music generaton.