Deep Generative Models

Lecture 12

Roman Isachenko

Moscow Institute of Physics and Technology

2022

Recap of previous lecture

Let take some pretrained image classification model to get the conditional label distribution $p(y|\mathbf{x})$ (e.g. ImageNet classifier).

Evaluation of likelihood-free models

- Sharpness $\Rightarrow$ low $H(y|\mathbf{x}) = -\sum_y \int_{\mathbf{x}} p(y, \mathbf{x}) \log p(y|\mathbf{x}) d\mathbf{x}$.
- Diversity $\Rightarrow$ high $H(y) = -\sum_y p(y) \log p(y)$.

Inception Score

$$IS = \exp(H(y) - H(y|\mathbf{x})) = \exp\left(\mathbb{E}_{\mathbf{x}} KL(p(y|\mathbf{x})||p(y))\right)$$

Frechet Inception Distance

$$D^2(\pi, p) = \|\mathbf{m}_\pi - \mathbf{m}_p\|_2^2 + \mathrm{Tr}\left(\mathbf{\Sigma}_\pi + \mathbf{\Sigma}_p - 2\sqrt{\mathbf{\Sigma}_\pi \mathbf{\Sigma}_p}\right).$$

FID is related to moment matching.

Salimans T. et al. Improved Techniques for Training GANs, 2016
Heusel M. et al. GANs Trained by a Two Time-Scale Update Rule Converge to a Local Nash Equilibrium, 2017

Recap of previous lecture

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

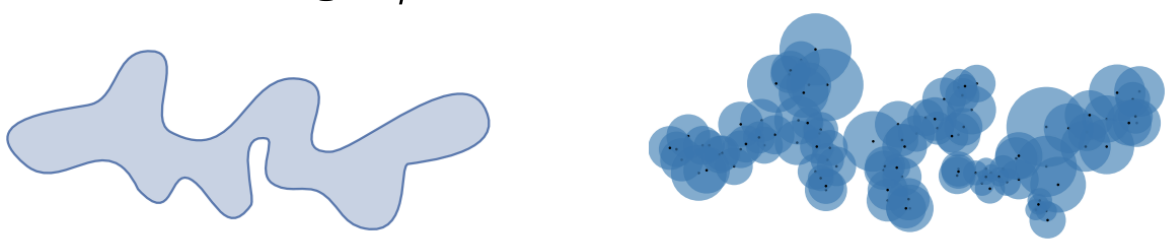
Embed samples using pretrained classifier network (as previously):

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

Define binary function:

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

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



(a) True manifold (b) Approx. manifold

Kynkäänniemi T. et al. Improved precision and recall metric for assessing generative models, 2019

Recap of previous lecture

Discrete VAE latents

- Define dictionary (word book) space $\{\mathbf{e}_k\}_{k=1}^K$, where $\mathbf{e}_k \in \mathbb{R}^C$, K is the size of the dictionary.
- Our variational posterior $q(c|\mathbf{x}, \phi) = \text{Categorical}(\boldsymbol{\pi}(\mathbf{x}, \phi))$ (encoder) outputs discrete probabilities vector.
- We sample c^* from $q(c|\mathbf{x}, \phi)$ (reparametrization trick analogue).
- Our generative distribution $p(\mathbf{x}|\mathbf{e}_{c^*}, \boldsymbol{\theta})$ (decoder).

ELBO

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

KL term

$$KL(q(c|\mathbf{x}, \phi)||p(c)) = -H(q(c|\mathbf{x}, \phi)) + \log K.$$

Is it possible to make reparametrization trick? (we sample from discrete distribution now!).

Outline

1. Discrete VAE latent representations
   - Vector quantization
   - Gumbel-softmax

2. Neural ODE

Outline

1. Discrete VAE latent representations
   - Vector quantization
   - Gumbel-softmax
2. Neural ODE

Outline

Vector quantization

Quantized representation

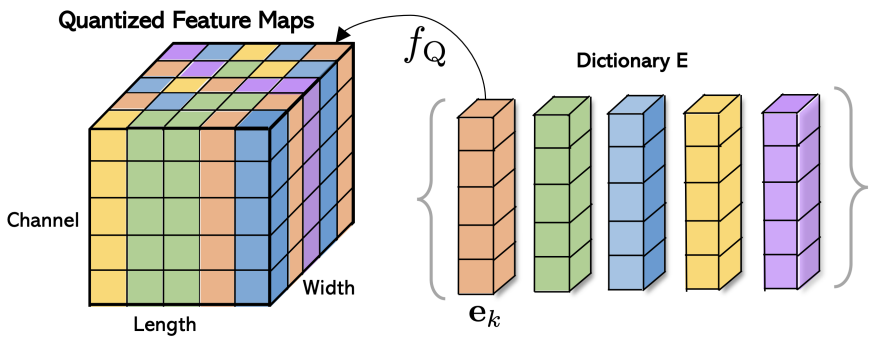
$\mathbf{z}_q \in \mathbb{R}^C$ for $\mathbf{z} \in \mathbb{R}^C$ is defined by a nearest neighbor look-up using the shared dictionary space

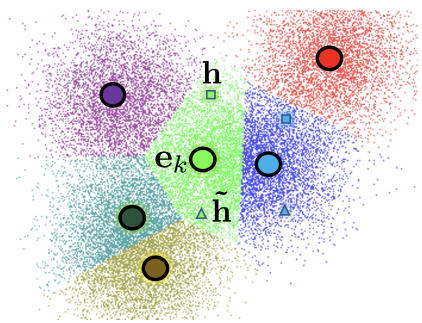
$$\mathbf{z}_q = \mathbf{e}_{k^*}, \quad \text{where } k^* = \arg\min_k \|\mathbf{z} - \mathbf{e}_k\|.$$

- Let our encoder outputs continuous representation $\mathbf{z}$.
- Quantization will give us the discrete distribution $q(c|\mathbf{x}, \phi)$.

Quantization procedure

If we have tensor with the spatial dimensions we apply the quantization for each of $W \times H$ locations.





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

Vector Quantized VAE (VQ-VAE)

Let VAE latent variable $\mathbf{c} \in \{1, \dots, K\}^{W \times H}$ is the discrete with spatial-independent variational posterior and prior distributions

$$q(\mathbf{c}|\mathbf{x}, \phi) = \prod_{i=1}^{W} \prod_{j=1}^{H} q(c_{ij}|\mathbf{x}, \phi); \quad p(\mathbf{c}) = \prod_{i=1}^{W} \prod_{j=1}^{H} \text{Uniform}\{1, \dots, K\}.$$

Let $\mathbf{z}_e = \text{NN}_e(\mathbf{x}, \phi) \in \mathbb{R}^{W \times H \times C}$ is the encoder output.

Deterministic variational posterior

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

$KL(q(c|\mathbf{x}, \phi)||p(c))$ term in ELBO is constant, entropy of the posterior is zero.

$$KL(q(c|\mathbf{x}, \phi)||p(c)) = -H(q(c|\mathbf{x}, \phi)) + \log K = \log K.$$

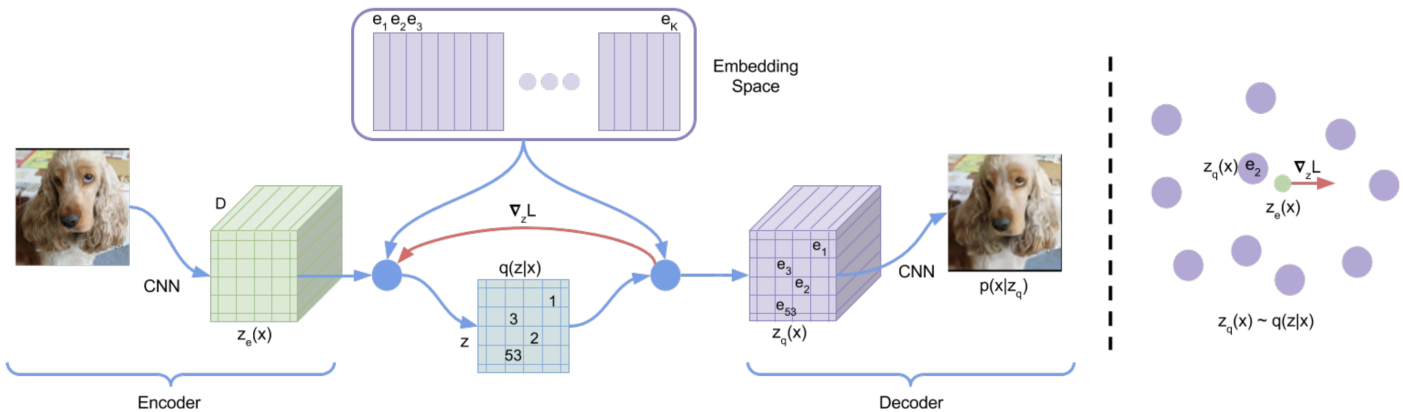
Oord A., Vinyals O., Kavukcuoglu K. Neural Discrete Representation Learning, 2017

Vector Quantized VAE (VQ-VAE)

ELBO

$$\mathcal{L}(\phi, \theta) = \mathbb{E}_{q(c|\mathbf{x},\phi)} \log p(\mathbf{x}|\mathbf{e}_c, \theta) - \log K = \log p(\mathbf{x}|\mathbf{z}_q, \theta) - \log K,$$

where $z_q = \mathbf{e}_{k^*}$, $k^* = \arg\min_k \|\mathbf{z}_e - \mathbf{e}_k\|$.



Problem: arg min is not differentiable.

Straight-through gradient estimation

$$\frac{\partial \log p(\mathbf{x}|\mathbf{z}_q, \theta)}{\partial \phi} = \frac{\partial \log p(\mathbf{x}|\mathbf{z}_q, \theta)}{\partial \mathbf{z}_q} \cdot \frac{\partial \mathbf{z}_q}{\partial \phi} \approx \frac{\partial \log p(\mathbf{x}|\mathbf{z}_q, \theta)}{\partial \mathbf{z}_q} \cdot \frac{\partial \mathbf{z}_e}{\partial \phi}$$

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

Vector Quantized VAE-2 (VQ-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

Outline

Gumbel-softmax trick

- VQ-VAE has deterministic variational posterior (it allows to get rid of discrete sampling and reparametrization trick).
- There is no uncertainty in the encoder output.

Gumbel-max trick

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

$$c = \arg\max_k [\log \pi_k + g_k],$$

has a categorical distribution $c \sim \text{Categorical}(\boldsymbol{\pi})$.

- Let our encoder $q(c|\mathbf{x}, \boldsymbol{\phi}) = \text{Categorical}(\boldsymbol{\pi}(\mathbf{x}, \boldsymbol{\phi}))$ outputs logits of $\boldsymbol{\pi}(\mathbf{x}, \boldsymbol{\phi})$.
- We could sample from the discrete distribution using Gumbel-max reparametrization.

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

Gumbel-softmax trick

Reparametrization trick (LOTUS)

$$\nabla_\phi \mathbb{E}_{q(c|\mathbf{x},\phi)} \log p(\mathbf{x}|\mathbf{e}_c, \boldsymbol{\theta}) = \mathbb{E}_{\text{Gumbel}(0,1)} \nabla_\phi \log p(\mathbf{x}|\mathbf{e}_{k^*}, \boldsymbol{\theta}),$$

where $k^* = \arg\max_k [\log q(k|\mathbf{x}, \phi) + g_k]$.

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

Gumbel-softmax relaxation

Concrete distribution = **con**tinuous + dis**crete**

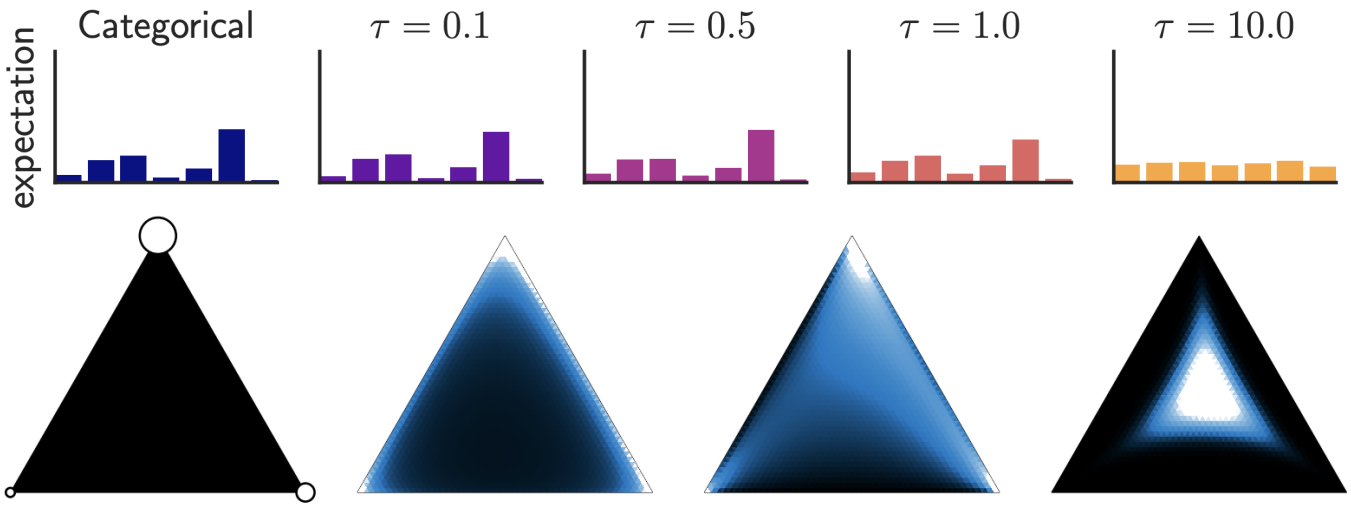
$$\hat{c}_k = \frac{\exp\left(\frac{\log q(k|\mathbf{x},\phi)+g_k}{\tau}\right)}{\sum_{j=1}^{K} \exp\left(\frac{\log q(j|\mathbf{x},\phi)+g_j}{\tau}\right)}, \quad k = 1, \ldots, K.$$

Here τ is a temperature parameter. Now we have differentiable operation, but the gradient estimate is biased now.

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

Gumbel-softmax trick

Concrete distribution



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

Reparametrization trick

$$\nabla_\phi \mathbb{E}_{q(c|\mathbf{x},\phi)} \log p(\mathbf{x}|\mathbf{e}_c, \boldsymbol{\theta}) = \mathbb{E}_{\text{Gumbel}(0,1)} \nabla_\phi \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}),$$

where $\mathbf{z} = \sum_{k=1}^{K} \hat{c}_k \mathbf{e}_k$ (all operations are differentiable now).

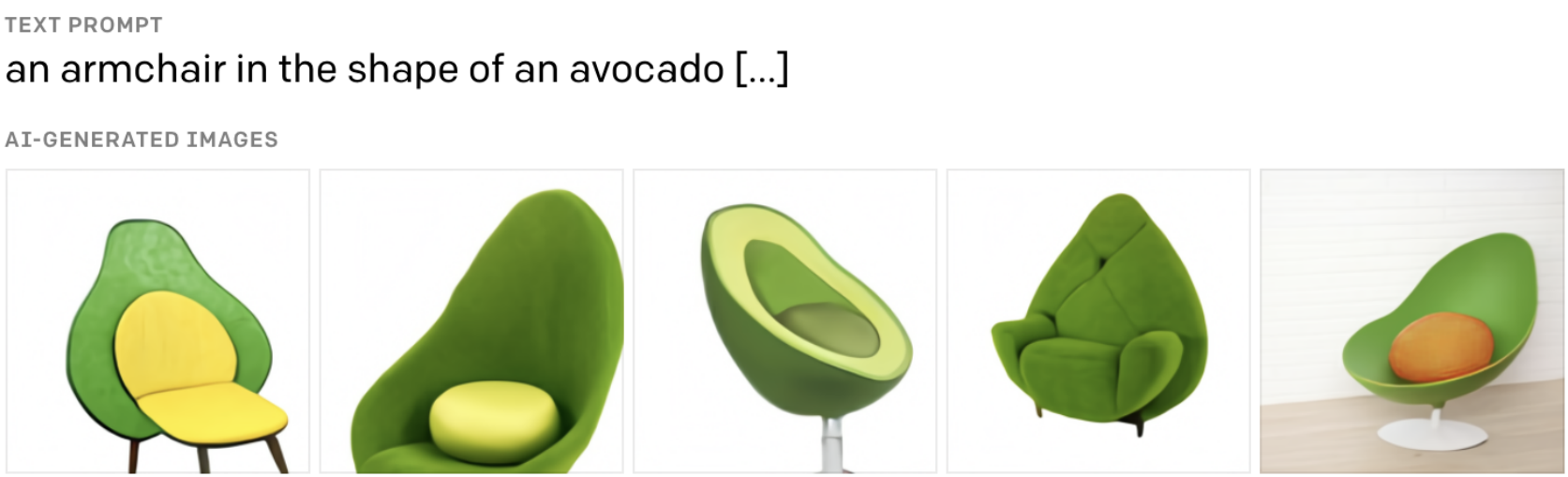
Maddison C. J., Mnih A., Teh Y. W. The Concrete distribution: A continuous relaxation of discrete random variables, 2016
Jang E., Gu S., Poole B. Categorical reparameterization with Gumbel-Softmax, 2016

DALL-E/dVAE

Deterministic VQ-VAE posterior

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

- Gumbel-Softmax trick allows to make true categorical distribution and sample from it.
- Since latent space is discrete we could train autoregressive transformers in it.
- It is a natural way to incorporate text and image token spaces.



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

Outline

Neural ODE

Consider Ordinary Differential Equation (ODE)

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

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

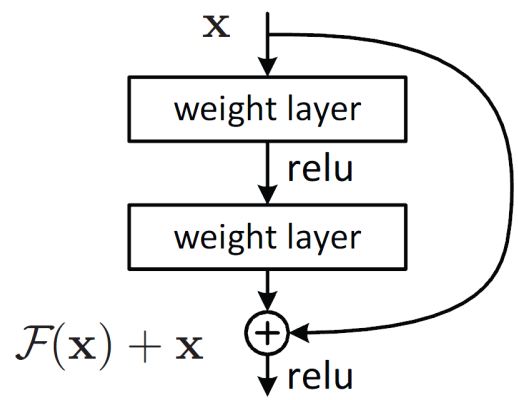
Euler update step

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

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

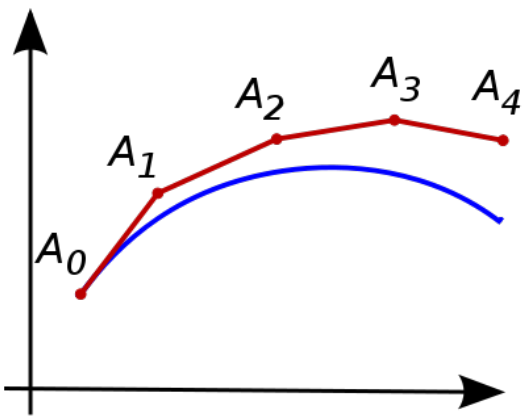
Neural ODE

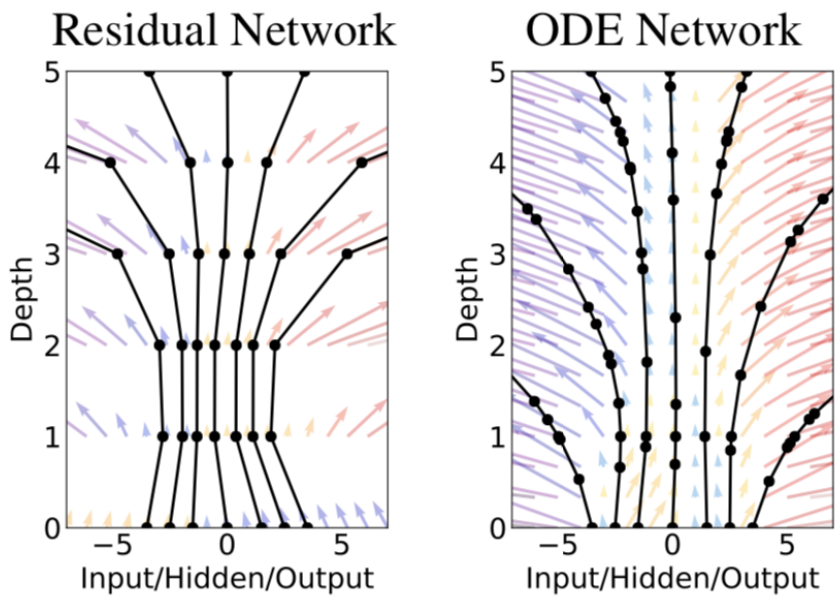
Residual block

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

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)

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

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)

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

Do we know any initilal condition?

Solution for adjoint function

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

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

Note: These equations are solved back in time.

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

Neural ODE

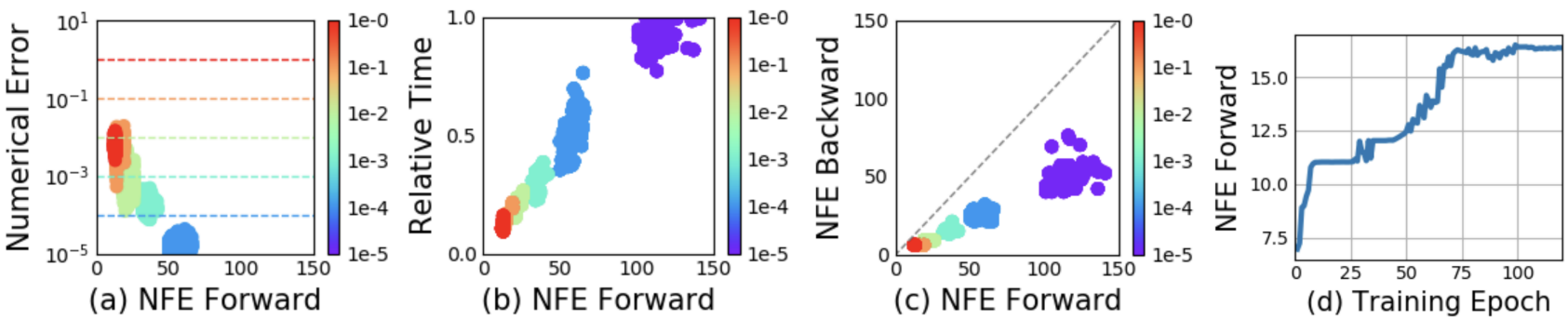
Forward pass

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

Backward pass

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

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



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

Summary

- Vector Quantization is the way to create VAE with discrete latent space and deterministic variational posterior.
- Straight-through gradient ignores quantize operation in backprop.
- Gumbel-softmax trick relaxes discrete problem to continuous one using Gumbel-max reparametrization trick.
- It becomes more and more popular to use discrete latent spaces in the fields of image/video/music generation.
- 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.