Deep Generative Models

Lecture 9

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AI Masters

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Recap of previous lecture

f-divergence minimization

$$D_f(\pi||p) = \mathbb{E}_{p(\mathbf{x})} f\left(\frac{\pi(\mathbf{x})}{p(\mathbf{x})}\right) \to \min_p .$$

Here $f : \mathbb{R}_+ \to \mathbb{R}$ is a convex, lower semicontinuous function satisfying $f(1) = 0$.

Variational divergence estimation

$$D_f(\pi||p) \geq \sup_{T \in \mathcal{T}} \left[\mathbb{E}_\pi T(\mathbf{x}) - \mathbb{E}_p f^*(T(\mathbf{x}))\right],$$

Fenchel conjugate

$$f^*(t) = \sup_{u \in \text{dom}_f} (ut - f(u)), \quad f(u) = \sup_{t \in \text{dom}_{f*}} (ut - f^*(t))$$

Note: To evaluate lower bound we only need samples from $\pi(\mathbf{x})$ and $p(\mathbf{x})$. Hence, we could fit implicit generative model.

Nowozin S., Cseke B., Tomioka R. f-GAN: Training Generative Neural Samplers using Variational Divergence Minimization, 2016

Recap of previous lecture

How to evaluate likelihood-free models?

$p(y|\mathbf{x})$ – pretrained image classification model (e.g. ImageNet classifier).

What do we want from samples?

- **Sharpness**

Low sharpness

High sharpness

  $p(y|\mathbf{x})$ has low entropy (each image $\mathbf{x}$ should have distinctly recognizable object).

- **Diversity**

Low diversity

High diversity

  $p(y) = \int p(y|\mathbf{x})p(\mathbf{x})d\mathbf{x}$ has high entropy (there should be as many classes generated as possible).

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image credit: https://deepgenerativemodels.github.io

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

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

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.

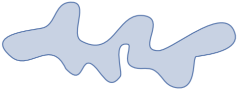
Embed samples using pretrained classifier network (as previously):

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

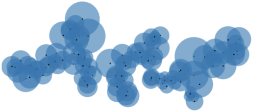
Define binary function:

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

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



(a) True manifold



(b) Approx. manifold

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

Outline

1. Neural ODE
2. Adjoint method
3. Continuous-in-time Normalizing Flows

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1. Neural ODE
2. Adjoint method
3. Continuous-in-time Normalizing Flows

Neural ODE

Consider Ordinary Differential Equation (ODE)

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

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

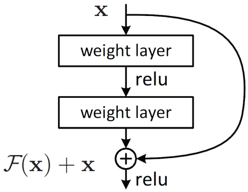
Euler update step

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

Residual block

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

- 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

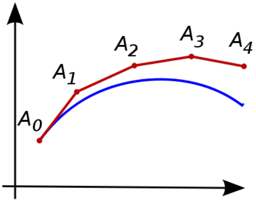
Neural ODE

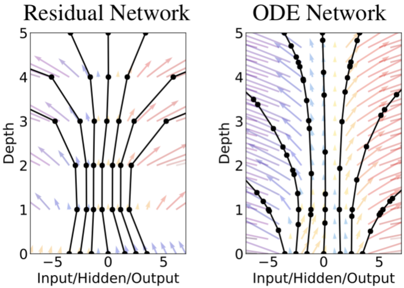
Residual block

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

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:

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





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

Neural ODE

Forward pass (loss function)

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

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

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2. Adjoint method

3. Continuous-in-time Normalizing Flows

Adjoint method

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)

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

Do we know any initilal condition?

Solution for adjoint function

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

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

Note: These equations are solved back in time.

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Adjoint method

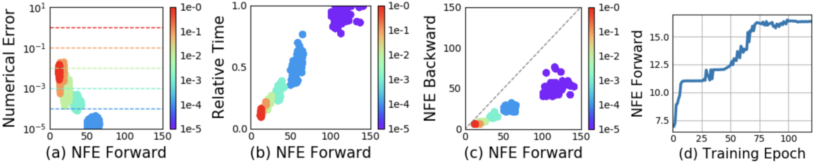
Forward pass

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

Backward pass

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

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



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2. Adjoint method
3. Continuous-in-time Normalizing Flows

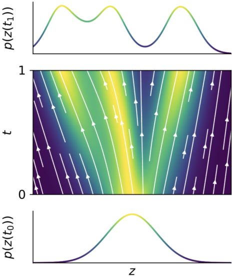
Continuous-in-time Normalizing Flows

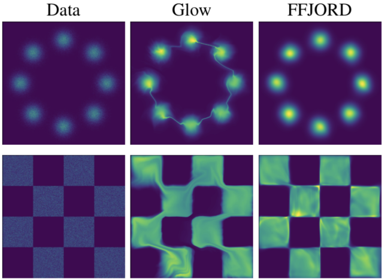
Discrete-in-time NF

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

Continuous-in-time dynamics

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





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

Continuous-in-time Normalizing Flows

Theorem (Picard)

If f is uniformly Lipschitz continuous in $\mathbf{z}$ and continuous in t, then the ODE has a **unique** solution.

Note: Unlike discrete-in-time NF, f does not need to be bijective (uniqueness guarantees bijectivity).

- Discrete-in-time NF need invertible f. Here we have sequence of $\log p(\mathbf{z}_t)$.
- Continuous-in-time NF require only smoothness of f. Here we need to get $\log(p(\mathbf{z}(t), t))$

Forward and inverse transforms

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

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

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

Continuous-in-time Normalizing Flows

Theorem (Kolmogorov-Fokker-Planck: special case)

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

$$\frac{d \log p(\mathbf{z}(t), t)}{dt} = -\mathrm{tr}\left(\frac{\partial f_{\boldsymbol{\theta}}(\mathbf{z}(t), t)}{\partial \mathbf{z}(t)}\right).$$

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

Here $p(\mathbf{x}|\boldsymbol{\theta}) = p(\mathbf{z}(t_1), t_1)$, $p(\mathbf{z}) = p(\mathbf{z}(t_0), t_0)$. **Adjoint** method is used for getting the derivatives.

Forward transform + log-density

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

It costs $O(m^2)$ to get the trace of the Jacobian (evaluation of determinant of the Jacobian costs $O(m^3)$!).

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

Continuous-in-time Normalizing Flows

- $\text{tr}\left(\frac{\partial f_{\boldsymbol{\theta}}(\mathbf{z}(t))}{\partial \mathbf{z}(t)}\right)$ costs $O(m^2)$ (m evaluations of f), since we have to compute a derivative for each diagonal element.
- Jacobian vector products $\mathbf{v}^T \frac{\partial f}{\partial \mathbf{z}}$ can be computed for approximately the same cost as evaluating f.

It is possible to reduce cost from $O(m^2)$ to $O(m)$!

Hutchinson's trace estimator

If $\boldsymbol{\epsilon} \in \mathbb{R}^m$ is a random variable with $\mathbb{E}[\boldsymbol{\epsilon}] = 0$ and $\text{Cov}(\boldsymbol{\epsilon}) = I$, then

$$\text{tr}(\mathbf{A}) = \text{tr}\left(\mathbf{A}\mathbb{E}_{p(\boldsymbol{\epsilon})}\left[\boldsymbol{\epsilon}\boldsymbol{\epsilon}^T\right]\right) = \mathbb{E}_{p(\boldsymbol{\epsilon})}\left[\text{tr}\left(\mathbf{A}\boldsymbol{\epsilon}\boldsymbol{\epsilon}^T\right)\right] = \mathbb{E}_{p(\boldsymbol{\epsilon})}\left[\boldsymbol{\epsilon}^T\mathbf{A}\boldsymbol{\epsilon}\right]$$

FFJORD density estimation

$$\log p(\mathbf{z}(t_1)) = \log p(\mathbf{z}(t_0)) - \int_{t_0}^{t_1} \text{tr}\left(\frac{\partial f_{\boldsymbol{\theta}}(\mathbf{z}(t), t)}{\partial \mathbf{z}(t)}\right) dt =$$

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

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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.
- Kolmogorov-Fokker-Planck theorem allows to construct continuous-in-time normalizing flow with less functional restrictions.
- FFJORD model makes such kind of NF scalable.