Deep Generative Models

Lecture 12

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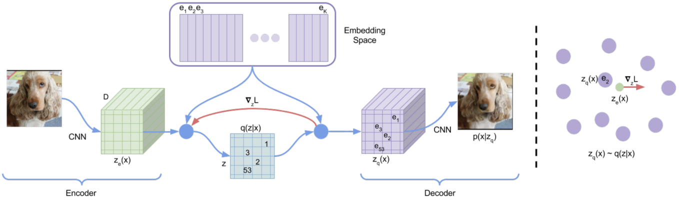
Recap of previous lecture



Deterministic variational posterior

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

ELBO

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

Straight-through gradient estimation

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

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

Recap of previous lecture

Gumbel-max trick

Let $g_k \sim \text{Gumbel}(0, 1)$ for $k = 1, \dots, K$. Then

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

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

Gumbel-softmax relaxation

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

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

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

Recap of previous lecture

Consider Ordinary Differential Equation

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

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

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 equivalent to Euler update step for solving ODE with $\Delta t = 1$!

In the limit of adding more layers and taking smaller steps we get:

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

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

Recap of previous lecture

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

Outline

1. Neural ODE
2. Continuous-in-time normalizing flows
3. Langevin dynamic and SDE basics

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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)

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

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

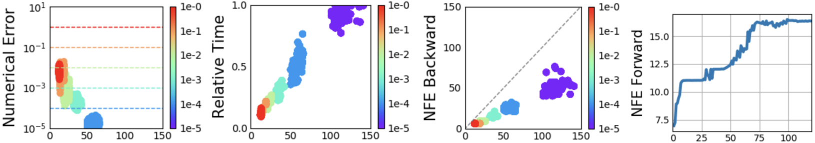
Forward pass

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

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.



(a) NFE Forward (b) NFE Forward (c) NFE Forward (d) Training Epoch

Outline

1. Neural ODE

2. Continuous-in-time normalizing flows

3. Langevin dynamic and SDE basics

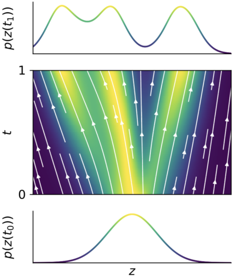
Continuous-in-time Normalizing Flows

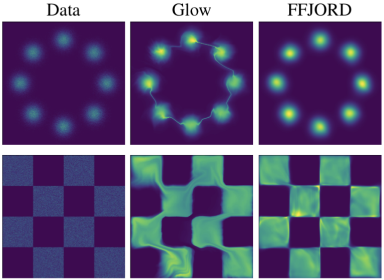
Discrete-in-time NF

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

Continuous-in-time dynamics

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





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 flows, f does not need to be bijective (uniqueness guarantees bijectivity).

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

Forward and inverse transforms

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

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

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

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

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

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

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

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

- $\text{tr}\left(\frac{\partial f(\mathbf{z}(t),\boldsymbol{\theta})}{\partial \mathbf{z}(t)}\right)$ 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

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

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

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

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Langevin dynamic

Imagine that we have some generative model $p(\mathbf{x}|\boldsymbol{\theta})$.

Statement

Let $\mathbf{x}_0$ be a random vector. Then under mild regularity conditions for small enough η samples from the following dynamics

$$\mathbf{x}_{t+1} = \mathbf{x}_t + \eta \frac{1}{2} \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\boldsymbol{\theta}) + \sqrt{\eta} \cdot \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, 1).$$

will comes from $p(\mathbf{x}|\boldsymbol{\theta})$.

What do we get if $\boldsymbol{\epsilon} = \mathbf{0}$?

Energy-based model

$$p(\mathbf{x}|\boldsymbol{\theta}) = \frac{\hat{p}(\mathbf{x}|\boldsymbol{\theta})}{Z_{\boldsymbol{\theta}}}, \quad \text{where } Z_{\boldsymbol{\theta}} = \int \hat{p}(\mathbf{x}|\boldsymbol{\theta}) d\mathbf{x}$$

$$\nabla_{\mathbf{x}} \log p(\mathbf{x}|\boldsymbol{\theta}) = \nabla_{\mathbf{x}} \log \hat{p}(\mathbf{x}|\boldsymbol{\theta}) - \nabla_{\mathbf{x}} \log Z_{\boldsymbol{\theta}} = \nabla_{\mathbf{x}} \log \hat{p}(\mathbf{x}|\boldsymbol{\theta})$$

Gradient of normalized density equals to gradient of unnormalized density.

Welling M. Bayesian Learning via Stochastic Gradient Langevin Dynamics, 2011

Stochastic differential equation (SDE)

Let define stochastic process $\mathbf{x}(t)$ with initial condition $\mathbf{x}(0) \sim p_0(\mathbf{x})$:

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$$

- $\mathbf{f}(\mathbf{x}, t)$ is the **drift** function of $\mathbf{x}(t)$.
- $g(t)$ is the **diffusion** coefficient of $\mathbf{x}(t)$.
- If $g(t) = 0$ we get standard ODE.
- $\mathbf{w}(t)$ is the standard Wiener process (Brownian motion)

$$\mathbf{w}(t) - \mathbf{w}(s) \sim \mathcal{N}(0, t-s), \quad d\mathbf{w} = \boldsymbol{\epsilon} \cdot \sqrt{dt}, \text{ where } \boldsymbol{\epsilon} \sim \mathcal{N}(0, 1).$$

How to get distribution $p(\mathbf{x}, t)$ for $\mathbf{x}(t)$?

Theorem (Kolmogorov-Fokker-Planck)

Evolution of the distribution $p(\mathbf{x}, t)$ is given by the following ODE:

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} = \mathrm{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\big[\mathbf{f}(\mathbf{x}, t)p(\mathbf{x}, t)\big] + \frac{1}{2}g^2(t)\frac{\partial^2 p(\mathbf{x}, t)}{\partial \mathbf{x}^2}\right)$$

Stochastic differential equation (SDE)

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}, \quad d\mathbf{w} = \boldsymbol{\epsilon} \cdot \sqrt{dt}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, 1).$$

Langevin SDE (special case)

$$d\mathbf{x} = \frac{1}{2}\frac{\partial}{\partial \mathbf{x}} \log p(\mathbf{x}, t)dt + 1 d\mathbf{w}$$

Langevin discrete dynamic

$$\mathbf{x}_{t+1} = \mathbf{x}_t + \eta \frac{1}{2}\frac{\partial}{\partial \mathbf{x}} \log p(\mathbf{x}|\boldsymbol{\theta}) + \sqrt{\eta} \cdot \boldsymbol{\epsilon}, \quad \eta \approx dt.$$

Let apply KFP theorem.

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} = \mathrm{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\left[p(\mathbf{x}, t)\frac{1}{2}\frac{\partial}{\partial \mathbf{x}} \log p(\mathbf{x}, t)\right] + \frac{1}{2}\frac{\partial^2 p(\mathbf{x}, t)}{\partial \mathbf{x}^2}\right) =$$

$$= \mathrm{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\left[\frac{1}{2}\frac{\partial}{\partial \mathbf{x}} p(\mathbf{x}, t)\right] + \frac{1}{2}\frac{\partial^2 p(\mathbf{x}, t)}{\partial \mathbf{x}^2}\right) = 0$$

The density $p(\mathbf{x}, t) = \text{const}$.

Summary

- 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 flows scalable.
- Langevin dynamics allows to sample from the model using the score function (due to the existence of stationary distribution for SDE).