Deep Generative Models

Lecture 3

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AI Masters

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Recap of previous lecture

Jacobian matrix

Let $f : \mathbb{R}^m \to \mathbb{R}^m$ be a differentiable function.

$$\mathbf{z} = f(\mathbf{x}), \quad \mathbf{J} = \frac{\partial \mathbf{z}}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial z_1}{\partial x_1} & \cdots & \frac{\partial z_1}{\partial x_m} \\ \cdots & \cdots & \cdots \\ \frac{\partial z_m}{\partial x_1} & \cdots & \frac{\partial z_m}{\partial x_m} \end{pmatrix} \in \mathbb{R}^{m \times m}$$

Change of variable theorem (CoV)

Let $\mathbf{x}$ be a random variable with density function $p(\mathbf{x})$ and $f : \mathbb{R}^m \to \mathbb{R}^m$ is a differentiable, invertible function (diffeomorphism). If $\mathbf{z} = f(\mathbf{x})$, $\mathbf{x} = f^{-1}(\mathbf{z}) = g(\mathbf{z})$, then

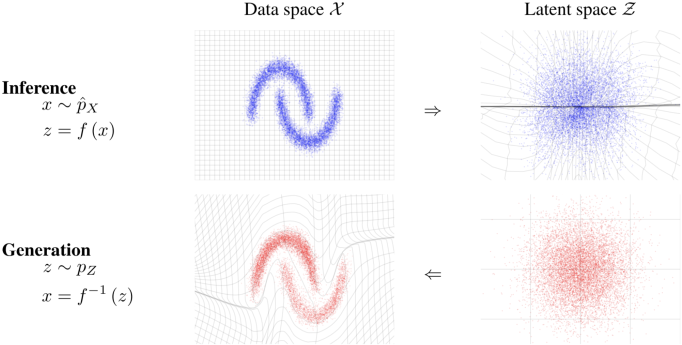
$$p(\mathbf{x}) = p(\mathbf{z})|\det(\mathbf{J}_f)| = p(\mathbf{z}) \left|\det\left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}}\right)\right| = p(f(\mathbf{x})) \left|\det\left(\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}}\right)\right|$$

$$p(\mathbf{z}) = p(\mathbf{x})|\det(\mathbf{J}_g)| = p(\mathbf{x}) \left|\det\left(\frac{\partial \mathbf{x}}{\partial \mathbf{z}}\right)\right| = p(g(\mathbf{z})) \left|\det\left(\frac{\partial g(\mathbf{z})}{\partial \mathbf{z}}\right)\right|.$$

Recap of previous lecture

Definition

Normalizing flow is a *differentiable, invertible* mapping from data $\mathbf{x}$ to the noise $\mathbf{z}$.



Log likelihood

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(f_K \circ \dots \circ f_1(\mathbf{x})) + \sum_{k=1}^{K} \log |\det(\mathbf{J}_{f_k})|$$

Dinh L., Sohl-Dickstein J., Bengio S. Density estimation using Real NVP, 2016

Recap of previous lecture

Forward KL for flow model

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(f_{\boldsymbol{\theta}}(\mathbf{x})) + \log |\det(\mathbf{J}_f)|$$

Reverse KL for flow model

$$KL(p||\pi) = \mathbb{E}_{p(\mathbf{z})} \left[\log p(\mathbf{z}) - \log |\det(\mathbf{J}_g)| - \log \pi(g_{\boldsymbol{\theta}}(\mathbf{z})) \right]$$

Flow KL duality

$$\arg\min_{\boldsymbol{\theta}} KL(\pi(\mathbf{x})||p(\mathbf{x}|\boldsymbol{\theta})) = \arg\min_{\boldsymbol{\theta}} KL(p(\mathbf{z}|\boldsymbol{\theta})||p(\mathbf{z}))$$

- $p(\mathbf{z})$ is a base distribution; $\pi(\mathbf{x})$ is a data distribution;
- $\mathbf{z} \sim p(\mathbf{z})$, $\mathbf{x} = g_{\boldsymbol{\theta}}(\mathbf{z})$, $\mathbf{x} \sim p(\mathbf{x}|\boldsymbol{\theta})$;
- $\mathbf{x} \sim \pi(\mathbf{x})$, $\mathbf{z} = f_{\boldsymbol{\theta}}(\mathbf{x})$, $\mathbf{z} \sim p(\mathbf{z}|\boldsymbol{\theta})$.

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

Recap of previous lecture

Flow log-likelihood

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log p(f_{\boldsymbol{\theta}}(\mathbf{x})) + \log |\det(\mathbf{J}_f)|$$

The main challenge is a determinant of the Jacobian.

Linear flows

$$\mathbf{z} = f_{\boldsymbol{\theta}}(\mathbf{x}) = \mathbf{W}\mathbf{x}, \quad \mathbf{W} \in \mathbb{R}^{m \times m}, \quad \boldsymbol{\theta} = \mathbf{W}, \quad \mathbf{J}_f = \mathbf{W}^T$$

- LU-decomposition
$$\mathbf{W} = \mathbf{P}\mathbf{L}\mathbf{U}.$$
- QR-decomposition
$$\mathbf{W} = \mathbf{Q}\mathbf{R}.$$

Decomposition should be done only once in the beggining. Next, we fit decomposed matrices ($\mathbf{P}/\mathbf{L}/\mathbf{U}$ or $\mathbf{Q}/\mathbf{R}$).

Kingma D. P., Dhariwal P. Glow: Generative Flow with Invertible 1x1 Convolutions, 2018
Hoogeboom E., et al. Emerging convolutions for generative normalizing flows, 2019

Recap of previous lecture

Consider an autoregressive model

$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{j=1}^{m} p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta}), \quad p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta}) = \mathcal{N}\left(\mu_j(\mathbf{x}_{1:j-1}), \sigma_j^2(\mathbf{x}_{1:j-1})\right).$$

Gaussian autoregressive NF

$$\mathbf{x} = g_{\boldsymbol{\theta}}(\mathbf{z}) \quad \Rightarrow \quad x_j = \sigma_j(\mathbf{x}_{1:j-1}) \cdot z_j + \mu_j(\mathbf{x}_{1:j-1}).$$

$$\mathbf{z} = f_{\boldsymbol{\theta}}(\mathbf{x}) \quad \Rightarrow \quad z_j = (x_j - \mu_j(\mathbf{x}_{1:j-1})) \cdot \frac{1}{\sigma_j(\mathbf{x}_{1:j-1})}.$$

- We have an **invertible** and **differentiable** transformation from $p(\mathbf{z})$ to $p(\mathbf{x}|\boldsymbol{\theta})$.
- Jacobian of such transformation is triangular!

Generation function $g_{\boldsymbol{\theta}}(\mathbf{z})$ is **sequential**.
Inference function $f_{\boldsymbol{\theta}}(\mathbf{x})$ is **not sequential**.

Papamakarios G., Pavlakou T., Murray I. Masked Autoregressive Flow for Density Estimation, 2017

Outline

1. RealNVP: coupling layer
2. Neural ODE
3. Adjoint method
4. Continuous-in-time Normalizing Flows

Outline

1. RealNVP: coupling layer
2. Neural ODE
3. Adjoint method
4. Continuous-in-time Normalizing Flows

RealNVP

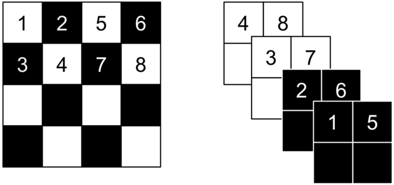
Let split $\mathbf{x}$ and $\mathbf{z}$ in two parts:

$$\mathbf{x} = [\mathbf{x}_1, \mathbf{x}_2] = [\mathbf{x}_{1:d}, \mathbf{x}_{d+1:m}]; \quad \mathbf{z} = [\mathbf{z}_1, \mathbf{z}_2] = [\mathbf{z}_{1:d}, \mathbf{z}_{d+1:m}].$$

Coupling layer

$$\begin{cases} \mathbf{x}_1 = \mathbf{z}_1; \\ \mathbf{x}_2 = \mathbf{z}_2 \odot \boldsymbol{\sigma}_\theta(\mathbf{z}_1) + \boldsymbol{\mu}_\theta(\mathbf{z}_1). \end{cases} \qquad \begin{cases} \mathbf{z}_1 = \mathbf{x}_1; \\ \mathbf{z}_2 = (\mathbf{x}_2 - \boldsymbol{\mu}_\theta(\mathbf{x}_1)) \odot \frac{1}{\boldsymbol{\sigma}_\theta(\mathbf{x}_1)}. \end{cases}$$

Image partitioning



- Checkerboard ordering uses masking.
- Channelwise ordering uses splitting.

Dinh L., Sohl-Dickstein J., Bengio S. Density estimation using Real NVP, 2016

RealNVP

Coupling layer

$$\begin{cases} \mathbf{x}_1 = \mathbf{z}_1; \\ \mathbf{x}_2 = \mathbf{z}_2 \odot \boldsymbol{\sigma}_{\boldsymbol{\theta}}(\mathbf{z}_1) + \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z}_1). \end{cases} \qquad \begin{cases} \mathbf{z}_1 = \mathbf{x}_1; \\ \mathbf{z}_2 = (\mathbf{x}_2 - \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{x}_1)) \odot \frac{1}{\boldsymbol{\sigma}_{\boldsymbol{\theta}}(\mathbf{x}_1)}. \end{cases}$$

Estimating the density takes 1 pass, sampling takes 1 pass!

Jacobian

$$\det \left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) = \det \begin{pmatrix} \mathbf{I}_d & 0_{d \times m-d} \\ \frac{\partial \mathbf{z}_2}{\partial \mathbf{x}_1} & \frac{\partial \mathbf{z}_2}{\partial \mathbf{x}_2} \end{pmatrix} = \prod_{j=1}^{m-d} \frac{1}{\sigma_j(\mathbf{x}_1)}.$$

Gaussian AR NF

$$\mathbf{x} = g_{\boldsymbol{\theta}}(\mathbf{z}) \quad \Rightarrow \quad x_j = \sigma_j(\mathbf{x}_{1:j-1}) \cdot z_j + \mu_j(\mathbf{x}_{1:j-1}).$$

$$\mathbf{z} = f_{\boldsymbol{\theta}}(\mathbf{x}) \quad \Rightarrow \quad z_j = (x_j - \mu_j(\mathbf{x}_{1:j-1})) \cdot \frac{1}{\sigma_j(\mathbf{x}_{1:j-1})}.$$

How to get RealNVP coupling layer from gaussian AR NF?

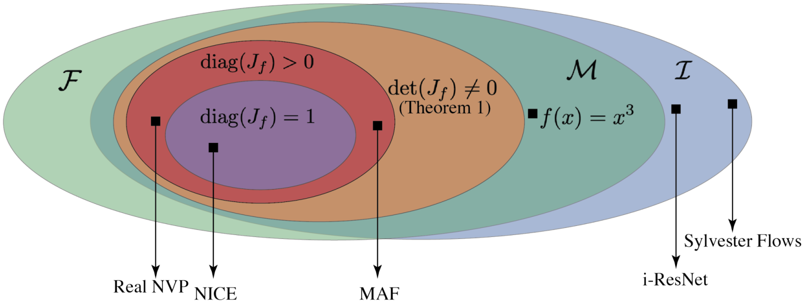
Dinh L., Sohl-Dickstein J., Bengio S. Density estimation using Real NVP, 2016

Glow samples

Glow model: coupling layer + linear flows (1x1 convs)

Kingma D. P., Dhariwal P. Glow: Generative Flow with Invertible 1x1 Convolutions, 2018

Venn diagram for Normalizing flows



- $\mathcal{I}$ – invertible functions.
- $\mathcal{F}$ – continuously differentiable functions whose Jacobian is lower triangular.
- $\mathcal{M}$ – invertible functions from $\mathcal{F}$.

Song Y., Meng C., Ermon S. Mintnet: Building invertible neural networks with masked convolutions, 2019

Outline

Neural ODE

Consider Ordinary Differential Equation (ODE)

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

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

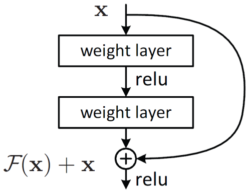
Euler update step

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

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

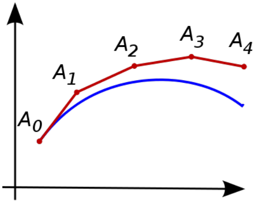
Neural ODE

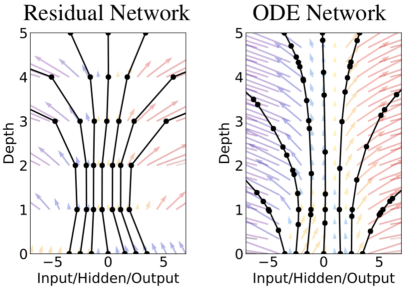
Residual block

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

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

Outline

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.

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

Adjoint method

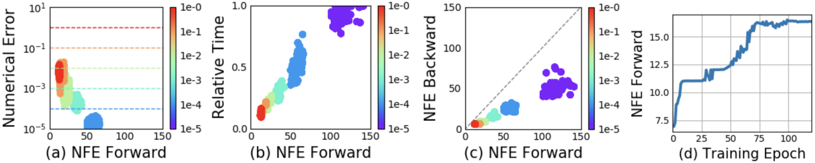
Forward pass

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

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.



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

Outline

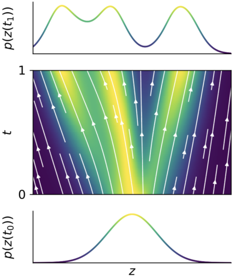
Continuous-in-time Normalizing Flows

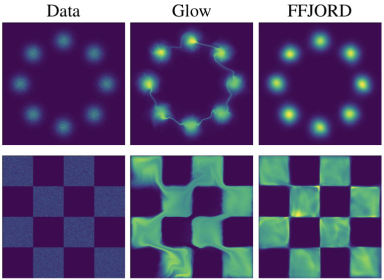
Discrete-in-time NF

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

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

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

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

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

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

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

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

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

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

Summary

- The RealNVP coupling layer is an effective type of flow (special case of AR flows) that has fast inference and generation modes.
- 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.