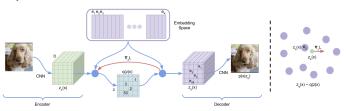
# Deep Generative Models

Lecture 13

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#### 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**

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

## Straight-through gradient estimation

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

#### Gumbel-max trick

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

$$c = \argmax_k [\log \pi_k + g_k]$$

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

#### 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

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

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

Consider Ordinary Differential Equation

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

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

Euler update step

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

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  $\Delta t = 1$ ! In the limit of adding more layers and taking smaller steps we get:

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

$$\mathbf{a_z}(t) = \frac{\partial L(\mathbf{y})}{\partial \mathbf{z}(t)}; \quad \mathbf{a_{\theta}}(t) = \frac{\partial L(\mathbf{y})}{\partial \theta(t)}$$
 - adjoint functions.

Theorem (Pontryagin)

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

Forward pass

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

Backward pass

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

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

## Outline

1. Continuous-in-time normalizing flows

2. Langevin dynamic and SDE basics

3. Score matching

# Outline

1. Continuous-in-time normalizing flows

Langevin dynamic and SDE basics

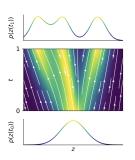
3. Score matching

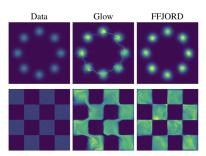
#### Discrete-in-time NF

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

## Continuous-in-time dynamics

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





# 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).

#### Forward and inverse transforms

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

# Theorem (Kolmogorov-Fokker-Planck: special case)

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

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

#### Density evaluation

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

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

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

- ▶ Discrete-in-time normalizing flows need invertible f. It costs  $O(m^3)$  to get determinant of the Jacobian.
- Continuous-in-time flows require only smoothness of f. It costs  $O(m^2)$  to get the trace of the Jacobian.

- ▶  $\operatorname{tr}\left(\frac{\partial f(\mathbf{z}(t),\theta)}{\partial \mathbf{z}(t)}\right)$  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  $\epsilon \in \mathbb{R}^m$  is a random variable with  $\mathbb{E}[\epsilon] = 0$  and  $\mathsf{Cov}(\epsilon) = I$ , then  $\mathsf{tr}(\mathbf{A}) = \mathsf{tr}(\mathbf{A}\mathbb{E}[\epsilon]) = \mathbb{E}[\epsilon] = 0$  and  $\mathsf{Tr}(\mathbf{A}) = \mathsf{tr}(\mathbf{A}) = \mathsf{tr}$ 

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

## FFJORD density estimation

$$\begin{split} \log p(\mathbf{z}(t_1)) &= \log p(\mathbf{z}(t_0)) - \int_{t_0}^{t_1} \operatorname{tr} \left( \frac{\partial f(\mathbf{z}(t), t, \boldsymbol{\theta})}{\partial \mathbf{z}(t)} \right) dt = \\ &= \log p(\mathbf{z}(t_0)) - \mathbb{E}_{p(\epsilon)} \int_{t_0}^{t_1} \left[ \epsilon^T \frac{\partial f}{\partial \mathbf{z}} \epsilon \right] dt. \end{split}$$

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

# Outline

1. Continuous-in-time normalizing flows

2. Langevin dynamic and SDE basics

3. Score matching

# Langevin dynamic

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

#### Statement

Let  $\mathbf{x}_0$  be a random vector. Then under mild regularity conditions for small enough  $\eta$  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  $\epsilon = \mathbf{0}$ ?

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.

# Stochastic differential equation (SDE)

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

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

- **f**( $\mathbf{x}$ , t) is the **drift** function of  $\mathbf{x}$ (t).
- ightharpoonup 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)

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

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:

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

# Stochastic differential equation (SDE)

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

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.

$$\begin{split} \frac{\partial p(\mathbf{x}, t)}{\partial t} &= \operatorname{tr} \left( -\frac{\partial}{\partial \mathbf{x}} \left[ p(\mathbf{x}, t) \frac{1}{2} \frac{\partial}{\partial \mathbf{x}} \log p(\mathbf{x}, t) \right] + \frac{1}{2} \frac{\partial^2 p(\mathbf{x}, t)}{\partial \mathbf{x}^2} \right) = \\ &= \operatorname{tr} \left( -\frac{\partial}{\partial \mathbf{x}} \left[ \frac{1}{2} \frac{\partial}{\partial \mathbf{x}} p(\mathbf{x}, t) \right] + \frac{1}{2} \frac{\partial^2 p(\mathbf{x}, t)}{\partial \mathbf{x}^2} \right) = 0 \end{split}$$

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

# Stochastic differential equation (SDE)

#### Statement

Let  $\mathbf{x}_0$  be a random vector. Then 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 come from  $p(\mathbf{x}|\boldsymbol{\theta})$  under mild regularity conditions for small enough  $\eta$  and large enough t.

The density  $p(\mathbf{x}|\theta)$  is a **stationary** distribution for this SDE.

Song Y. Generative Modeling by Estimating Gradients of the Data Distribution, blog post, 2021

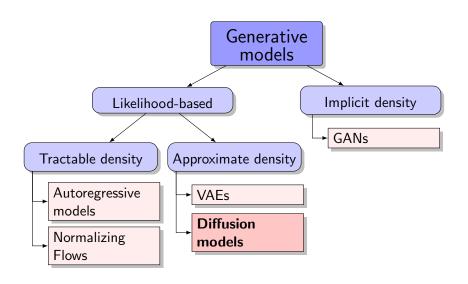
# Outline

1. Continuous-in-time normalizing flows

Langevin dynamic and SDE basics

3. Score matching

#### Generative models zoo



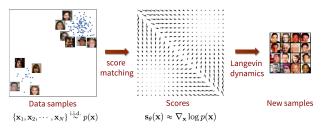
# Score matching

We could sample from the model using Langevin dynamics if we have  $\nabla_{\mathbf{x}} \log p(\mathbf{x}|\boldsymbol{\theta})$ .

#### Fisher divergence

$$D_{F}(\pi, p) = \frac{1}{2} \mathbb{E}_{\pi} \left\| \nabla_{\mathbf{x}} \log p(\mathbf{x}|\boldsymbol{\theta}) - \nabla_{\mathbf{x}} \log \pi(\mathbf{x}) \right\|_{2}^{2} \to \min_{\boldsymbol{\theta}}$$

Let introduce score function  $s(x, \theta) = \nabla_x \log \rho(x|\theta)$ .



**Problem:** we do not know  $\nabla_{\mathbf{x}} \log \pi(\mathbf{x})$ .

Song Y. Generative Modeling by Estimating Gradients of the Data Distribution, blog post, 2021

# Score matching

# Theorem (implicit score matching)

Under some regularity conditions, it holds

$$\frac{1}{2}\mathbb{E}_{\pi}\big\|\mathbf{s}(\mathbf{x},\boldsymbol{\theta}) - \nabla_{\mathbf{x}}\log\pi(\mathbf{x})\big\|_{2}^{2} = \mathbb{E}_{\pi}\Big[\frac{1}{2}\|\mathbf{s}(\mathbf{x},\boldsymbol{\theta})\|_{2}^{2} + \mathrm{tr}\big(\nabla_{\mathbf{x}}\mathbf{s}(\mathbf{x},\boldsymbol{\theta})\big)\Big] + \mathrm{const}$$

## Proof (only for 1D)

$$\mathbb{E}_{\pi} \| s(x) - \nabla_{x} \log \pi(x) \|_{2}^{2} = \mathbb{E}_{\pi} \left[ s(x)^{2} + (\nabla_{x} \log \pi(x))^{2} - 2[s(x)\nabla_{x} \log \pi(x)] \right]$$

$$\mathbb{E}_{\pi} [s(x)\nabla_{x} \log \pi(x)] = \int \pi(x)\nabla_{x} \log p(x)\nabla_{x} \log \pi(x) dx$$

$$= \int \nabla_{x} \log p(x)\nabla_{x}\pi(x) dx = \pi(x)\nabla_{x} \log p(x) \Big|_{-\infty}^{+\infty}$$

$$- \int \nabla_{x}^{2} \log p(x)\pi(x) dx = -\mathbb{E}_{\pi}\nabla_{x}^{2} \log p(x) = -\mathbb{E}_{\pi}\nabla_{x}s(x)$$

$$\frac{1}{2}\mathbb{E}_{\pi} \| s(x) - \nabla_{x} \log \pi(x) \|_{2}^{2} = \mathbb{E}_{\pi} \left[ \frac{1}{2}s(x)^{2} + \nabla_{x}s(x) \right] + \text{const.}$$

# Score matching

## Theorem (implicit score matching)

$$\frac{1}{2}\mathbb{E}_{\pi}\big\|\mathbf{s}(\mathbf{x},\boldsymbol{\theta}) - \nabla_{\mathbf{x}}\log\pi(\mathbf{x})\big\|_{2}^{2} = \mathbb{E}_{\pi}\Big[\frac{1}{2}\|\mathbf{s}(\mathbf{x},\boldsymbol{\theta})\|_{2}^{2} + \mathrm{tr}\big(\nabla_{\mathbf{x}}\mathbf{s}(\mathbf{x},\boldsymbol{\theta})\big)\Big] + \mathrm{const}$$

Here  $\nabla_{\mathbf{x}}\mathbf{s}(\mathbf{x}, \boldsymbol{\theta}) = \nabla_{\mathbf{x}}^2 \log p(\mathbf{x}|\boldsymbol{\theta})$  is a Hessian matrix.

- 1. The left hand side is intractable due to unknown  $\pi(\mathbf{x})$  denoising score matching.
- The right hand side is complex due to Hessian matrix sliced score matching.

Sliced score matching (Hutchinson's trace estimation)

$$\mathsf{tr}ig( 
abla_{\mathsf{x}} \mathsf{s}(\mathsf{x}, oldsymbol{ heta}) ig) = \mathbb{E}_{p(oldsymbol{\epsilon})} \left[ oldsymbol{\epsilon}^{\mathsf{T}} 
abla_{\mathsf{x}} \mathsf{s}(\mathsf{x}, oldsymbol{ heta}) oldsymbol{\epsilon} 
ight]$$

Song Y. Sliced Score Matching: A Scalable Approach to Density and Score Estimation, 2019

Song Y. Generative Modeling by Estimating Gradients of the Data Distribution, blog post, 2021

# Denoising score matching

Let perturb original data by normal noise  $p(\mathbf{x}|\mathbf{x}',\sigma) = \mathcal{N}(\mathbf{x}|\mathbf{x}',\sigma^2\mathbf{I})$ 

$$\pi(\mathbf{x}|\sigma) = \int \pi(\mathbf{x}') p(\mathbf{x}|\mathbf{x}',\sigma) d\mathbf{x}'.$$

Then the solution of

$$\frac{1}{2}\mathbb{E}_{\pi(\mathbf{x}|\sigma)}\big\|\mathbf{s}(\mathbf{x},\boldsymbol{\theta},\sigma) - \nabla_{\mathbf{x}}\log\pi(\mathbf{x}|\sigma)\big\|_2^2 \to \min_{\boldsymbol{\theta}}$$

satisfies  $\mathbf{s}(\mathbf{x}, \boldsymbol{\theta}, \sigma) \approx \mathbf{s}(\mathbf{x}, \boldsymbol{\theta}, 0) = \mathbf{s}(\mathbf{x}, \boldsymbol{\theta})$  if  $\sigma$  is small enough.

#### **Theorem**

$$\mathbb{E}_{\pi(\mathbf{x}|\sigma)} \|\mathbf{s}(\mathbf{x}, \boldsymbol{\theta}, \sigma) - \nabla_{\mathbf{x}} \log \pi(\mathbf{x}|\sigma)\|_{2}^{2} =$$

$$= \mathbb{E}_{\pi(\mathbf{x}')} \mathbb{E}_{p(\mathbf{x}|\mathbf{x}',\sigma)} \|\mathbf{s}(\mathbf{x}, \boldsymbol{\theta}, \sigma) - \nabla_{\mathbf{x}} \log p(\mathbf{x}|\mathbf{x}',\sigma)\|_{2}^{2} + \text{const}(\boldsymbol{\theta})$$

- Here  $\nabla_{\mathbf{x}} \log p(\mathbf{x}|\mathbf{x}', \sigma) = -\frac{\mathbf{x} \mathbf{x}'}{\sigma^2}$ .
  - ► The RHS does not need to compute  $\nabla_{\mathbf{x}} \log \pi(\mathbf{x}|\sigma)$  and even more  $\nabla_{\mathbf{x}} \log \pi(\mathbf{x})$ .
  - **s**( $\mathbf{x}, \boldsymbol{\theta}, \sigma$ ) tries to **denoise** a corrupted sample.
  - ▶ Score function  $\mathbf{s}(\mathbf{x}, \boldsymbol{\theta}, \sigma)$  parametrized by  $\sigma$ . How to make it?

# Summary

- 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).
- Score matching proposes to minimize Fisher divergence to get score function.
- Sliced score matching and denoising score matching are two techniques to get scalable algorithm for fitting Fisher divergence.