Deep Generative Models

Lecture 13

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Recap of previous lecture

Training of DDPM

1. Get the sample $\mathbf{x}_0 \sim \pi(\mathbf{x})$.
2. Sample timestamp $t \sim U\{1, T\}$ and the noise $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$.
3. Get noisy image $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon}$.
4. Compute loss $\mathcal{L}_{\text{simple}} = \|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t)\|^2$.

Sampling of DDPM

1. Sample $\mathbf{x}_T \sim \mathcal{N}(0, \mathbf{I})$.
2. Compute mean of $p(\mathbf{x}_{t-1}|\mathbf{x}_t, \boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\mu}_{\boldsymbol{\theta},t}(\mathbf{x}_t), \sigma_t^2 \cdot \mathbf{I})$:

$$\boldsymbol{\mu}_{\boldsymbol{\theta},t}(\mathbf{x}_t) = \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{\alpha_t(1 - \bar{\alpha}_t)}} \cdot \boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t)$$

3. Get denoised image $\mathbf{x}_{t-1} = \boldsymbol{\mu}_{\boldsymbol{\theta},t}(\mathbf{x}_t) + \sigma_t \cdot \boldsymbol{\epsilon}$, where $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$.

Ho J. Denoising Diffusion Probabilistic Models, 2020

Recap of previous lecture

DDPM objective

$$\mathbb{E}_{\pi(\mathbf{x}_0)}\mathbb{E}_{t\sim U\{1,T\}}\mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)}\left[\frac{(1-\alpha_t)^2}{2\tilde{\beta}_t\alpha_t}\left\|\mathbf{s}_{\boldsymbol{\theta},t}(\mathbf{x}_t)-\nabla_{\mathbf{x}_t}\log q(\mathbf{x}_t|\mathbf{x}_0)\right\|_2^2\right]$$

In practice the coefficient is omitted.

NCSN objective

$$\mathbb{E}_{\pi(\mathbf{x}_0)}\mathbb{E}_{t\sim U\{1,T\}}\mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)}\left\|\mathbf{s}_{\boldsymbol{\theta},\sigma_t}(\mathbf{x}_t)-\nabla_{\mathbf{x}_t}\log q(\mathbf{x}_t|\mathbf{x}_0)\right\|_2^2$$

Note: The objective of DDPM and NCSN is almost identical. But the difference in sampling scheme:

- NCSN uses annealed Langevin dynamics;
- DDPM uses ancestral sampling.

$$\mathbf{s}_{\boldsymbol{\theta},t}(\mathbf{x}_t)=-\frac{\boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t)}{\sqrt{1-\bar{\alpha}_t}}=\nabla_{\mathbf{x}_t}\log p(\mathbf{x}_t|\boldsymbol{\theta})$$

Ho J. Denoising Diffusion Probabilistic Models, 2020

Recap of previous lecture

Unconditional generation

$$\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t + \frac{1-\alpha_t}{\sqrt{\alpha_t}} \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\boldsymbol{\theta}) + \sigma_t \cdot \boldsymbol{\epsilon}$$

Conditional generation

$$\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t + \frac{1-\alpha_t}{\sqrt{\alpha_t}} \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y}, \boldsymbol{\theta}) + \sigma_t \cdot \boldsymbol{\epsilon}$$

Conditional distribution

$$\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y}, \boldsymbol{\theta}) = \nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t) - \frac{\boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t)}{\sqrt{1-\bar{\alpha}_t}}$$

Here $p(\mathbf{y}|\mathbf{x}_t)$ – classifier on noisy samples (we have to learn it separately).

Classifier-corrected noise prediction

$$\boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t, \mathbf{y}) = \boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t) - \sqrt{1-\bar{\alpha}_t} \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t)$$

Dhariwal P., Nichol A. Diffusion Models Beat GANs on Image Synthesis, 2021

Recap of previous lecture

Guidance scale

$$\boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t, \mathbf{y}) = \boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t) - \gamma \cdot \sqrt{1 - \bar{\alpha}_t} \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t)$$

$$\nabla^{\gamma}_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y}, \boldsymbol{\theta}) = \nabla_{\mathbf{x}_t} \log \left(\frac{p(\mathbf{y}|\mathbf{x}_t)^{\gamma} p(\mathbf{x}_t|\boldsymbol{\theta})}{Z} \right)$$

Note: Guidance scale γ tries to sharpen the distribution $p(\mathbf{y}|\mathbf{x}_t)$.

Guided sampling

$$\boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t, \mathbf{y}) = \boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t) - \gamma \cdot \sqrt{1 - \bar{\alpha}_t} \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t)$$

$$\boldsymbol{\mu}_{\boldsymbol{\theta},t}(\mathbf{x}_t, \mathbf{y}) = \frac{1}{\sqrt{\alpha_t}} \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{\alpha_t(1 - \bar{\alpha}_t)}} \cdot \boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t, \mathbf{y})$$

$$\mathbf{x}_{t-1} = \boldsymbol{\mu}_{\boldsymbol{\theta},t}(\mathbf{x}_t, \mathbf{y}) + \sigma_t \cdot \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$$

Dhariwal P., Nichol A. Diffusion Models Beat GANs on Image Synthesis, 2021

Recap of previous lecture

- Previous method requires training the additional classifier model $p(\mathbf{y}|\mathbf{x}_t)$ on the noisy data.
- Let try to avoid this requirement.

$$\nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t) = \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y}, \boldsymbol{\theta}) - \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\boldsymbol{\theta})$$

$$\nabla^{\gamma}_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y}, \boldsymbol{\theta}) = \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\boldsymbol{\theta}) + \gamma \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t) =$$
$$= (1 - \gamma) \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\boldsymbol{\theta}) + \gamma \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y}, \boldsymbol{\theta})$$

Classifier-free-corrected noise prediction

$$\hat{\boldsymbol{\epsilon}}_{\boldsymbol{\theta},t}(\mathbf{x}_t, \mathbf{y}) = \gamma \cdot \boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t, \mathbf{y}) + (1 - \gamma) \cdot \boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t)$$

- Train the single model $\boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t, \mathbf{y})$ on **supervised** data alternating with real conditioning $\mathbf{y}$ and empty conditioning $\mathbf{y} = \emptyset$.
- Apply the model twice during inference.

Ho J., Salimans T. Classifier-Free Diffusion Guidance, 2022

Outline

1. SDE basics
2. Diffusion and Score matching SDEs
3. Probability flow ODE

Outline

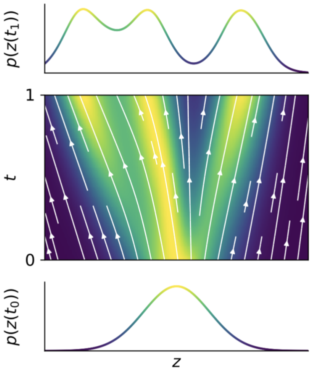
1. SDE basics
2. Diffusion and Score matching SDEs
3. Probability flow ODE

Ordinary differential equation (ODE)

Continuous-in-time Normalizing Flows

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

- Let $\mathbf{z}(t_0)$ will be a random variable with some density function $p(\mathbf{z}(t_0))$.
- Then $\mathbf{z}(t_1)$ will be also a random variable with some other density function $p(\mathbf{z}(t_1))$.
- We could say that we have the joint density function $p(\mathbf{z}(t), t)$.
- What is the difference between $p(\mathbf{z}(t), t)$ and $p(\mathbf{z}, t)$?



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

Ordinary differential equation (ODE)

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

Discretization of ODE (Euler method)

$$\mathbf{z}(t + dt) = \mathbf{z}(t) + \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{z}(t), t) \cdot dt$$

Theorem (Kolmogorov-Fokker-Planck: special case)

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

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

It means that if we have the value $\mathbf{z}_0 = \mathbf{z}(t_0)$ then the solution of the ODE will give us the density at the moment t_1.

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

Stochastic differential equation (SDE)

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

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

- $\mathbf{f}(\mathbf{x}, t) : \mathbb{R}^m \to \mathbb{R}^m$ is the **drift** function of $\mathbf{x}(t)$.
- $g(t) : \mathbb{R} \to \mathbb{R}$ is the **diffusion** function of $\mathbf{x}(t)$.
- If $g(t) = 0$ we get standard ODE.
- $\mathbf{w}(t)$ is the standard Wiener process (Brownian motion):
    1. $\mathbf{w}(0) = 0$ (almost surely);
    2. $\mathbf{w}(t)$ has independent increments;
    3. $\mathbf{w}(t) - \mathbf{w}(s) \sim \mathcal{N}(0, (t-s)\mathbf{I})$, for $t > s$.
- $d\mathbf{w} = \mathbf{w}(t + dt) - \mathbf{w}(t) = \mathcal{N}(0, \mathbf{I} \cdot dt) = \boldsymbol{\epsilon} \cdot \sqrt{dt}$, where $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$.

Stochastic differential equation (SDE)

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

- In contrast to ODE, initial condition $\mathbf{x}(0)$ does not uniquely determine the process trajectory.
- We have two sources of randomness: initial distribution $p_0(\mathbf{x})$ and Wiener process $w(t)$.

Discretization of SDE (Euler method)

$$\mathbf{x}(t + dt) = \mathbf{x}(t) + \mathbf{f}(\mathbf{x}(t), t) \cdot dt + g(t) \cdot \epsilon \cdot \sqrt{dt}$$

If $dt = 1$, then

$$\mathbf{x}_{t+1} = \mathbf{x}_t + \mathbf{f}(\mathbf{x}_t, t) + g(t) \cdot \epsilon$$

- At each moment t we have the density $p(\mathbf{x}(t), t)$.
- How to get the distribution $p(\mathbf{x}, t)$ for $\mathbf{x}(t)$?

Stochastic differential equation (SDE)

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

Theorem (Kolmogorov-Fokker-Planck)

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

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

Here

$$\mathrm{div}(\mathbf{v}) = \sum_{i=1}^{m} \frac{\partial v_i(\mathbf{x})}{\partial x_i} = \mathrm{tr}\left(\frac{\partial \mathbf{v}(\mathbf{x})}{\partial \mathbf{x}}\right)$$

$$\Delta_{\mathbf{x}} p(\mathbf{x}, t) = \sum_{i=1}^{m} \frac{\partial^2 p(\mathbf{x}, t)}{\partial x_i^2} = \mathrm{tr}\left(\frac{\partial^2 p(\mathbf{x}, t)}{\partial \mathbf{x}^2}\right)$$

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

Stochastic differential equation (SDE)

Theorem (Kolmogorov-Fokker-Planck)

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

- KFP theorem uniquely defines the dynamic $\mathbf{x}(t)$.
- This is the generalization of KFP theorem that we used in continuous-in-time NF:

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

Langevin SDE (special case)

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

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

Let apply KFP theorem.

Langevin SDE (special case)

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

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

The density $p(\mathbf{x}, t) = \mathrm{const}(t)$!
If $\mathbf{x}(0) \sim p_0(\mathbf{x})$, then $\mathbf{x}(t) \sim p_0(\mathbf{x})$.

Discretized Langevin SDE

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

Langevin dynamic

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

Outline

Score matching SDE

Denoising score matching

$$\mathbf{x}_l = \mathbf{x} + \sigma_l \cdot \boldsymbol{\epsilon}_l, \quad p(\mathbf{x}_l|\mathbf{x}, \sigma_l) = \mathcal{N}(\mathbf{x}, \sigma_l^2 \mathbf{I})$$

$$\mathbf{x}_{l-1} = \mathbf{x} + \sigma_{l-1} \cdot \boldsymbol{\epsilon}_{l-1}, \quad p(\mathbf{x}_{l-1}|\mathbf{x}, \sigma_{l-1}) = \mathcal{N}(\mathbf{x}, \sigma_{l-1}^2 \mathbf{I})$$

$$\mathbf{x}_l = \mathbf{x}_{l-1} + \sqrt{\sigma_l^2 - \sigma_{l-1}^2} \cdot \boldsymbol{\epsilon}, \quad p(\mathbf{x}_l|\mathbf{x}_{l-1}, \sigma_l) = \mathcal{N}(\mathbf{x}_{l-1}, (\sigma_l^2 - \sigma_{l-1}^2) \cdot \mathbf{I})$$

Let turn this Markov chain to the continuous stochastic process $\mathbf{x}(t)$ taking $L \to \infty$:

$$\mathbf{x}(t + dt) = \mathbf{x}(t) + \sqrt{\frac{\sigma^2(t + dt) - \sigma^2(t)}{dt} dt} \cdot \boldsymbol{\epsilon} = \mathbf{x}(t) + \sqrt{\frac{d[\sigma^2(t)]}{dt}} \cdot d\mathbf{w}$$

Variance Exploding SDE

$$d\mathbf{x} = \sqrt{\frac{d[\sigma^2(t)]}{dt}} \cdot d\mathbf{w}$$

Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Diffusion SDE

Denoising Diffusion

$$\mathbf{x}_t = \sqrt{1-\beta_t} \cdot \mathbf{x}_{t-1} + \sqrt{\beta_t} \cdot \boldsymbol{\epsilon}, \quad q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N}(\sqrt{1-\beta_t} \cdot \mathbf{x}_{t-1}, \beta_t \cdot \mathbf{I})$$

Let turn this Markov chain to the continuous stochastic process taking $T \to \infty$ and taking $\beta(\frac{t}{T}) = \beta_t \cdot T$

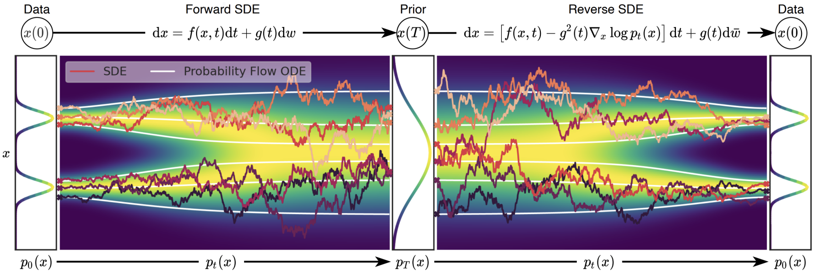
$$\begin{aligned} \mathbf{x}(t) &= \sqrt{1-\beta(t)dt} \cdot \mathbf{x}(t-dt) + \sqrt{\beta(t)dt} \cdot \boldsymbol{\epsilon} \approx \\ &\approx (1 - \frac{1}{2}\beta(t)dt) \cdot \mathbf{x}(t-dt) + \sqrt{\beta(t)dt} \cdot \boldsymbol{\epsilon} = \\ &= \mathbf{x}(t-dt) - \frac{1}{2}\beta(t)\mathbf{x}(t-dt)dt + \sqrt{\beta(t)} \cdot d\mathbf{w} \end{aligned}$$

Variance Preserving SDE

$$d\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}(t)dt + \sqrt{\beta(t)} \cdot d\mathbf{w}$$

Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Diffusion SDE



Variance Exploding SDE (NCSN)

$$d\mathbf{x} = \sqrt{\frac{d[\sigma^2(t)]}{dt}} \cdot d\mathbf{w}$$

Variance Preserving SDE (DDPM)

$$d\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}(t)dt + \sqrt{\beta(t)} \cdot d\mathbf{w}$$

Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Outline

1. SDE basics

2. Diffusion and Score matching SDEs

3. Probability flow ODE

Probability flow ODE

Theorem

Assume SDE $d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$ induces the distribution $p(\mathbf{x}, t)$. Then there exists ODE with identical probabilities distribution $p(\mathbf{x}, t)$ of the form

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

Proof

$$\begin{aligned}
\frac{\partial p(\mathbf{x}, t)}{\partial t} &= \text{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\big[\mathbf{f}(\mathbf{x}, t)p(\mathbf{x}, t)\big] + \frac{1}{2}g^2(t)\frac{\partial^2 p(\mathbf{x}, t)}{\partial \mathbf{x}^2}\right) = \\
&= \text{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\left[\mathbf{f}(\mathbf{x}, t)p(\mathbf{x}, t) + \frac{1}{2}g^2(t)\frac{\partial p(\mathbf{x}, t)}{\partial \mathbf{x}}\right]\right) = \\
&= \text{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\left[\mathbf{f}(\mathbf{x}, t)p(\mathbf{x}, t) + \frac{1}{2}g^2(t)p(\mathbf{x}, t)\frac{\partial \log p(\mathbf{x}, t)}{\partial \mathbf{x}}\right]\right) = \\
&= \text{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\left[\left(\mathbf{f}(\mathbf{x}, t) + \frac{1}{2}g^2(t)\frac{\partial \log p(\mathbf{x}, t)}{\partial \mathbf{x}}\right)p(\mathbf{x}, t)\right]\right)
\end{aligned}$$

Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Probability flow ODE

Theorem

Assume SDE $d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$ induces the distribution $p(\mathbf{x}, t)$. Then there exists ODE with identical probabilities distribution $p(\mathbf{x}, t)$ of the form

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

Proof (continued)

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

$$d\mathbf{x} = \tilde{\mathbf{f}}(\mathbf{x}, t)dt + 0 \cdot d\mathbf{w} = \left[\mathbf{f}(\mathbf{x}, t) - \frac{1}{2}g^2(t)\frac{\partial}{\partial \mathbf{x}} \log p(\mathbf{x}, t)\right] dt$$

Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Probability flow ODE

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

$$d\mathbf{x} = \left[\mathbf{f}(\mathbf{x}, t) - \frac{1}{2}g^2(t)\frac{\partial}{\partial \mathbf{x}}\log p(\mathbf{x}, t)\right] dt \text{ – Probability flow ODE}$$

Theorem (Kolmogorov-Fokker-Planck)

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

Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Probability flow ODE

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

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

Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Summary

- Score matching (NCSN) and diffusion models (DDPM) are the discretizations of the SDEs (variance exploding and variance preserving).