Deep Generative Models

Lecture 13

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AI Masters

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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. Probability flow ODE
3. Reverse SDE
4. Diffusion and Score matching SDEs

Outline

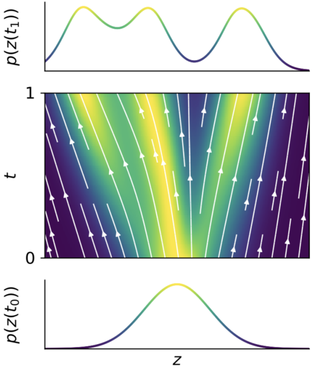
1. SDE basics
2. Probability flow ODE
3. Reverse SDE
4. Diffusion and Score matching SDEs

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

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

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 $\mathbf{x}(0) \sim p_0(\mathbf{x}) = \pi(\mathbf{x})$:

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

- $\mathbf{f}(\mathbf{x}, t) : \mathbb{R}^m \times [0, 1] \to \mathbb{R}^m$ is the **drift** function of $\mathbf{x}(t)$.
- $g(t) : \mathbb{R} \to \mathbb{R}$ is the **diffusion** function of $\mathbf{x}(t)$.
- $\mathbf{w}(t)$ 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 $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$.
- If $g(t) = 0$ we get standard ODE.

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 $\mathbf{w}(t)$.

Discretization of SDE (Euler method)

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

If $dt = 1$, then

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

- At each moment t we have the density $p(\mathbf{x}(t), t)$.
- $p : \mathbb{R}^m \times [0, 1] \to \mathbb{R}_+$ is a **probability path** between $p_0(\mathbf{x})$ and $p_1(\mathbf{x})$.
- How to get the distribution path $p(\mathbf{x}, t)$ 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 equation:

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

Here

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

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

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

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 SDE.
- 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 to this SDE.

Langevin SDE (special case)

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

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

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

Probability flow ODE

Theorem

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

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

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)

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

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

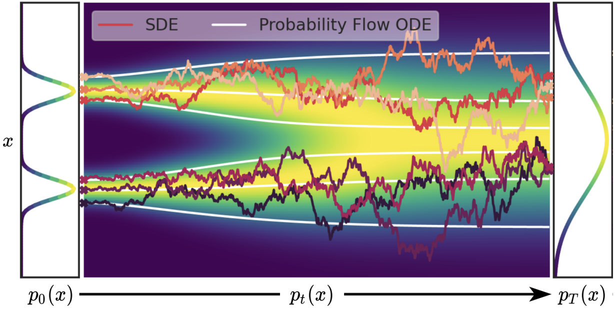
Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Probability flow ODE

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

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

- The term $\mathbf{s}(\mathbf{x}, t) = \frac{\partial}{\partial \mathbf{x}} \log p(\mathbf{x}, t)$ is a score function for continuous time.
- ODE has more stable trajectories.



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

Outline

Reverse SDE

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

Here dt could be > 0 or < 0.

Reverse ODE

Let $\tau = 1 - t$ ($d\tau = -dt$).

$$d\mathbf{x} = -\mathbf{f}(\mathbf{x}, 1 - \tau)d\tau$$

- How to revert SDE $d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$?
- Wiener process gives the randomness that we have to revert.

Theorem

There exists the reverse SDE for the SDE $d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$ that has the following form

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

with $dt < 0$.

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

Reverse SDE

Theorem

There exists the reverse SDE for the SDE $d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$ that has the following form

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

with $dt < 0$.

Note: Here we also see the score function $\mathbf{s}(\mathbf{x}, t) = \frac{\partial}{\partial \mathbf{x}} \log p(\mathbf{x}, t)$.

Sketch of the proof

- Convert initial SDE to probability flow ODE.
- Revert probability flow ODE.
- Convert reverse probability flow ODE to reverse SDE.

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

Reverse SDE

Proof

- Convert initial SDE to probability flow ODE

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

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

- Revert probability flow ODE

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

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

- Convert reverse probability flow ODE to reverse SDE

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

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

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

Reverse SDE

Theorem

There exists the reverse SDE for the SDE $d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$ that has the following form

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

with $dt < 0$.

Proof (continued)

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

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

Here $d\tau > 0$ and $dt < 0$.

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

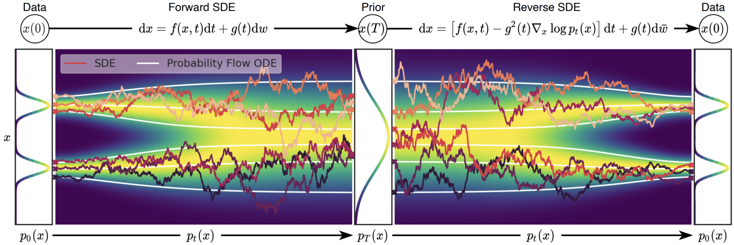
Reverse SDE

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

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

$$d\mathbf{x} = \left(\mathbf{f}(\mathbf{x}, t) - g^2(t)\frac{\partial \log p(\mathbf{x}, t)}{\partial \mathbf{x}}\right) dt + g(t)d\mathbf{w} \text{ -- reverse SDE}$$

- We got the way to transform one distribution to another via SDE with some probability path $p(\mathbf{x}, t)$.
- We are able to revert this process with the score function.



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

Outline

Score matching SDE

Denoising score matching

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

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

$$\mathbf{x}_t = \mathbf{x}_{t-1} + \sqrt{\sigma_t^2 - \sigma_{t-1}^2} \cdot \boldsymbol{\epsilon}, \quad q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_{t-1}, (\sigma_t^2 - \sigma_{t-1}^2) \cdot \mathbf{I})$$

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

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

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

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

Variance Exploding SDE (NCSN)

$$d\mathbf{x} = \sqrt{\frac{d[\sigma^2(t)]}{dt}} \cdot d\mathbf{w}, \quad \mathbf{f}(\mathbf{x}, t) = 0, \quad g(t) = \sqrt{\frac{d[\sigma^2(t)]}{dt}}$$

Variance grows since $\sigma(t)$ is a monotonically increasing function.

Variance Preserving SDE (DDPM)

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

$$\mathbf{f}(\mathbf{x}, t) = -\frac{1}{2}\beta(t)\mathbf{x}(t), \quad g(t) = \sqrt{\beta(t)}$$

Variance is preserved if $\mathbf{x}(0)$ has a unit variance.

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

Summary

- SDE defines stochastic process with drift and diffusion terms. ODEs are the special case of SDEs.
- KFP equation defines the dynamic of the probability function for the SDE.
- Langevin SDE has constant probability path.
- There exists special probability flow ODE for each SDE that gives the same probability path.
- It is possible to revert SDE using score function.
- Score matching (NCSN) and diffusion models (DDPM) are the discretizations of the SDEs (variance exploding and variance preserving).