Lecture 17 - Denoising Diffusion Model

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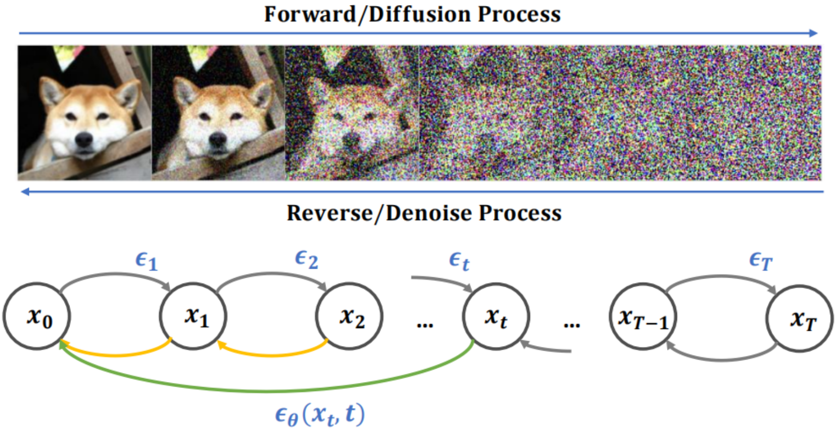
Denoising Diffusion Probabilistic Models, DDPM[1]



[1] Denoising diffusion probabilistic models. Advances in Neural Information Processing Systems, 33, 2020

Forward Diffusion Process

- 一步加噪过程

$$q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}) = \mathcal{N}(\boldsymbol{x}_t; \sqrt{\alpha_t}\boldsymbol{x}_{t-1}, (1-\alpha_t)\mathbf{I})$$

$$\mathbf{x}_t = \sqrt{\alpha_t}\mathbf{x}_{t-1} + \sqrt{(1-\alpha_t)}\boldsymbol{\epsilon}_{t-1}, \quad \text{where } \boldsymbol{\epsilon}_{t-1} \sim \mathcal{N}(0, \mathbf{I}).$$

- t步加噪过程

命题 1

条件分布$q(\boldsymbol{x}_t|\boldsymbol{x}_0)$为

$$q(\boldsymbol{x}_t|\boldsymbol{x}_0) = \mathcal{N}(\boldsymbol{x}_t; \sqrt{\overline{\alpha}_t}\boldsymbol{x}_0, (1-\overline{\alpha}_t)\mathbf{I}),$$

其中 $\overline{\alpha}_t = \prod_{i=1}^t \alpha_i$. 即 $\mathbf{x}_t = \sqrt{\overline{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\overline{\alpha}_t}\boldsymbol{\epsilon}_0$.

能够计算$q(\boldsymbol{x}_t|\boldsymbol{x}_0)$的好处在于给定$\boldsymbol{x}_0$，给一个$t$可以直接得到$\boldsymbol{x}_t$.

Proof

$$\begin{aligned}\mathbf{x}_t &= \sqrt{\alpha_t}\mathbf{x}_{t-1} + \sqrt{1-\alpha_t}\boldsymbol{\epsilon}_{t-1} \\ &= \sqrt{\alpha_t}(\sqrt{\alpha_{t-1}}\mathbf{x}_{t-2} + \sqrt{1-\alpha_{t-1}}\boldsymbol{\epsilon}_{t-2}) + \sqrt{1-\alpha_t}\boldsymbol{\epsilon}_{t-1} \\ &= \sqrt{\alpha_t\alpha_{t-1}}\mathbf{x}_{t-2} + \underbrace{\sqrt{\alpha_t}\sqrt{1-\alpha_{t-1}}\boldsymbol{\epsilon}_{t-2} + \sqrt{1-\alpha_t}\boldsymbol{\epsilon}_{t-1}}_{\mathbf{w}_1}.\end{aligned}$$

由于$\boldsymbol{\epsilon}_{t-2}$和$\boldsymbol{\epsilon}_{t-1}$都是标准高斯的，$\mathbf{w}_1$是均值为0的高斯，我们下面计算协方差

$$\begin{aligned}\mathbb{E}[\mathbf{w}_1\mathbf{w}_1^T] &= [(\sqrt{\alpha_t}\sqrt{1-\alpha_{t-1}})^2 + (\sqrt{1-\alpha_t})^2]\mathbf{I} \\ &= [\alpha_t(1-\alpha_{t-1}) + 1 - \alpha_t]\mathbf{I} = [1-\alpha_t\alpha_{t-1}]\mathbf{I}.\end{aligned}$$

延用记号$\boldsymbol{\epsilon}_t$

$$\begin{aligned}\mathbf{x}_t &= \sqrt{\alpha_t\alpha_{t-1}}\mathbf{x}_{t-2} + \sqrt{1-\alpha_t\alpha_{t-1}}\boldsymbol{\epsilon}_{t-2} \\ &= \sqrt{\alpha_t\alpha_{t-1}\alpha_{t-2}}\mathbf{x}_{t-3} + \sqrt{1-\alpha_t\alpha_{t-1}\alpha_{t-2}}\boldsymbol{\epsilon}_{t-3} \\ &= \cdots = \sqrt{\prod_{i=1}^{t}\alpha_i}\mathbf{x}_0 + \sqrt{1-\prod_{i=1}^{t}\alpha_i}\boldsymbol{\epsilon}_0.\end{aligned}$$

Reverse Denoising Process

我们希望用一个神经网络实现降噪过程，即

$$p_{\boldsymbol{\theta}}(\mathbf{x}_{t-1}|\mathbf{x}_t) \approx q(\mathbf{x}_{t-1}|\mathbf{x}_t)$$

由Markov性，

$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \frac{q(\mathbf{x}_{t-1}|\mathbf{x}_t)q(\mathbf{x}_t)}{q(\mathbf{x}_{t-1})} \xrightarrow{\text{condition on } \mathbf{x}_0} q(\mathbf{x}_t|\mathbf{x}_{t-1},\mathbf{x}_0) = \frac{q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)q(\mathbf{x}_t|\mathbf{x}_0)}{q(\mathbf{x}_{t-1}|\mathbf{x}_0)}$$

在优化神经网络的过程中转化为[2][3]

$$p_{\boldsymbol{\theta}}(\mathbf{x}_{t-1}|\mathbf{x}_t) \approx q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)$$

[2] Luo C. Understanding diffusion models: A unified perspective[J]. arXiv preprint arXiv:2208.11970, 2022.
[3] Chan S H. Tutorial on Diffusion Models for Imaging and Vision[J]. arXiv preprint arXiv:2403.18103, 2024.

Reverse Denoising Process

命题 2

条件分布$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$为一个高斯分布 $\mathcal{N}(\mathbf{x}_{t-1};\ \boldsymbol{\mu}_q(\mathbf{x}_t, \mathbf{x}_0), \boldsymbol{\Sigma}_q(t))$，其中

$$\mu_q(\mathbf{x}_t, \mathbf{x}_0) = \frac{(1-\overline{\alpha}_{t-1})\sqrt{\alpha_t}}{1-\overline{\alpha}_t}\mathbf{x}_t + \frac{(1-\alpha_t)\sqrt{\overline{\alpha}_{t-1}}}{1-\overline{\alpha}_t}\mathbf{x}_0$$

$$\boldsymbol{\Sigma}_q(t) = \frac{(1-\alpha_t)(1-\sqrt{\overline{\alpha}_{t-1}})}{1-\overline{\alpha}_t}\mathbf{I}$$

$$\begin{aligned} q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t, \boldsymbol{x}_0) &= \frac{q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}, \boldsymbol{x}_0)q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}{q(\boldsymbol{x}_t|\boldsymbol{x}_0)} \\ &= \frac{\mathcal{N}(\boldsymbol{x}_t; \sqrt{\alpha_t}\boldsymbol{x}_{t-1}, (1-\alpha_t)\mathbf{I})\mathcal{N}(\boldsymbol{x}_{t-1}; \sqrt{\bar{\alpha}_{t-1}}\boldsymbol{x}_0, (1-\bar{\alpha}_{t-1})\mathbf{I})}{\mathcal{N}(\boldsymbol{x}_t; \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0, (1-\bar{\alpha}_t)\mathbf{I})} \\ &\propto \exp\left\{-\left[\frac{(\boldsymbol{x}_t-\sqrt{\alpha_t}\boldsymbol{x}_{t-1})^2}{2(1-\alpha_t)} + \frac{(\boldsymbol{x}_{t-1}-\sqrt{\bar{\alpha}_{t-1}}\boldsymbol{x}_0)^2}{2(1-\bar{\alpha}_{t-1})} - \frac{(\boldsymbol{x}_t-\sqrt{\bar{\alpha}_t}\boldsymbol{x}_0)^2}{2(1-\bar{\alpha}_t)}\right]\right\} \end{aligned}$$

Reverse Denoising Process

注意到，给定加噪schedule，$\boldsymbol{\Sigma}_q(t)$是已知的，所以我们只需要参数化均值部分，即

$$p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t) = \mathcal{N}(\boldsymbol{x}_{t-1}; \boldsymbol{\mu}_{\boldsymbol{\theta}}, \boldsymbol{\Sigma}_q(t))$$

两个高斯分布之间的KL散度可以容易计算：

$$D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t, \boldsymbol{x}_0) \parallel p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)) = \frac{1}{2\sigma_q^2(t)} \left[\left\| \boldsymbol{\mu}_{\boldsymbol{\theta}} - \boldsymbol{\mu}_q \right\|_2^2 \right]$$

注意到

$$\begin{aligned} \boldsymbol{\mu}_q(\boldsymbol{x}_t, \boldsymbol{x}_0) &= \frac{(1-\overline{\alpha}_{t-1})\sqrt{\alpha_t}}{1-\overline{\alpha}_t}\boldsymbol{x}_t + \frac{(1-\alpha_t)\sqrt{\overline{\alpha}_{t-1}}}{1-\overline{\alpha}_t}\boldsymbol{x}_0 \\ &= \frac{(1-\overline{\alpha}_{t-1})\sqrt{\alpha_t}}{1-\overline{\alpha}_t}\boldsymbol{x}_t + \frac{(1-\alpha_t)\sqrt{\overline{\alpha}_{t-1}}}{1-\overline{\alpha}_t} \frac{\boldsymbol{x}_t - \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_0}{\sqrt{\bar{\alpha}_t}} \\ &= \frac{1}{\sqrt{\alpha_t}}\boldsymbol{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}\sqrt{\alpha_t}}\boldsymbol{\epsilon}_0 \end{aligned}$$

Denoising Diffusion Probabilistic Models

考虑

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

我们要学习的目标其实是一个 Denoiser $\boldsymbol{\epsilon}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t)$。

Algorithm 1 Training

```
repeat
  x_0 ~ q(x_0)
  t ~ Uniform({1, ..., T})
  ε ~ N(0, I)
  Take gradient descent step on
      ∇_θ ||ε − ε_θ(√ᾱ_t x_0 + √(1 − ᾱ_t) ε, t)||^2
until converged
```

$$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$$

Algorithm 2 Sampling

```
x_T ~ N(0, I)
for t = T, ..., 1 do
  z ~ N(0, I) if t > 1, else z = 0
  x_{t-1} = 1/√α_t (x_t − (1−α_t)/√(1−ᾱ_t) ε_θ(x_t, t)) + σ_t z
end for
return x_0
```

$$\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \sigma_t \mathbf{z}$$

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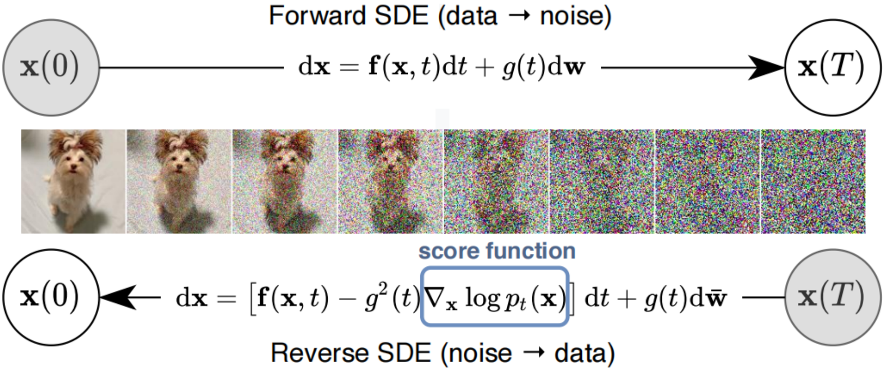
Score-based Generative Models, SGM[4]



[4] Y. Song, J. Sohl-Dickstein, D. P. Kingma, A. Kumar, S. Ermon, and B. Poole. Score-based generative modeling through stochastic differential equations. In Proc. ICLR, 2021.

Reverse SDE

定理 1

对于如下*SDE*:

$$\mathrm{d}\mathbf{x} = \mathbf{f}(\mathbf{x}, t)\mathrm{d}t + \mathbf{G}(\mathbf{x}, t)\mathrm{d}\mathbf{w}, \tag{1}$$

它的 *Reverse SDE* 为

$$\mathrm{d}\mathbf{x} = \{\mathbf{f}(\mathbf{x}, t) - \nabla \cdot [\mathbf{G}(\mathbf{x}, t)\mathbf{G}(\mathbf{x}, t)^{\top}] - \mathbf{G}(\mathbf{x}, t)\mathbf{G}(\mathbf{x}, t)^{\top}\nabla_{\mathbf{x}} \log p_t(\mathbf{x})\}\mathrm{d}t + \mathbf{G}(\mathbf{x}, t)\mathrm{d}\bar{\mathbf{w}}$$

Proof Sketch

SDE (1)的Fokker-Planck方程为

$$\frac{\partial p_t(\mathbf{x})}{\partial t} = -\sum_{i=1}^{d} \frac{\partial}{\partial x_i}[f_i(\mathbf{x},t)p_t(\mathbf{x})] + \frac{1}{2}\sum_{i=1}^{d}\sum_{j=1}^{d} \frac{\partial^2}{\partial x_i \partial x_j}\left[\sum_{k=1}^{d} G_{ik}(\mathbf{x},t)G_{jk}(\mathbf{x},t)p_t(\mathbf{x})\right]$$

$$= -\sum_{i=1}^{d} \frac{\partial}{\partial x_i}[f_i(\mathbf{x},t)p_t(\mathbf{x})] + \frac{1}{2}\sum_{i=1}^{d} \frac{\partial}{\partial x_i}\left[\sum_{j=1}^{d} \frac{\partial}{\partial x_j}\left[\sum_{k=1}^{d} G_{ik}(\mathbf{x},t)G_{jk}(\mathbf{x},t)p_t(\mathbf{x})\right]\right].$$

注意到

$$\sum_{j=1}^{d} \frac{\partial}{\partial x_j}\left[\sum_{k=1}^{d} G_{ik}(\mathbf{x},t)G_{jk}(\mathbf{x},t)p_t(\mathbf{x})\right]$$

$$= \sum_{j=1}^{d} \frac{\partial}{\partial x_j}\left[\sum_{k=1}^{d} G_{ik}(\mathbf{x},t)G_{jk}(\mathbf{x},t)\right] p_t(\mathbf{x}) + \sum_{j=1}^{d}\sum_{k=1}^{d} G_{ik}(\mathbf{x},t)G_{jk}(\mathbf{x},t)p_t(\mathbf{x})\frac{\partial}{\partial x_j}\log p_t(\mathbf{x})$$

$$= p_t(\mathbf{x})\nabla \cdot [\mathbf{G}(\mathbf{x},t)\mathbf{G}(\mathbf{x},t)^{\mathsf{T}}] + p_t(\mathbf{x})\mathbf{G}(\mathbf{x},t)\mathbf{G}(\mathbf{x},t)^{\mathsf{T}}\nabla_{\mathbf{x}} \log p_t(\mathbf{x})$$

Proof Sketch

回代Fokker-Planck方程

$$
\begin{aligned}
\frac{\partial p_t(\mathbf{x})}{\partial t} &= -\sum_{i=1}^{d} \frac{\partial}{\partial x_i}[f_i(\mathbf{x},t)p_t(\mathbf{x})] \\
&+ \frac{1}{2}\sum_{i=1}^{d} \frac{\partial}{\partial x_i}\Big[p_t(\mathbf{x})\nabla\cdot[\mathbf{G}(\mathbf{x},t)\mathbf{G}(\mathbf{x},t)^\mathsf{T}] + p_t(\mathbf{x})\mathbf{G}(\mathbf{x},t)\mathbf{G}(\mathbf{x},t)^\mathsf{T}\nabla_\mathbf{x}\log p_t(\mathbf{x})\Big] \\
&= -\sum_{i=1}^{d} \frac{\partial}{\partial x_i}\Big\{f_i(\mathbf{x},t)p_t(\mathbf{x}) \\
&- \frac{1}{2}\Big[\nabla\cdot[\mathbf{G}(\mathbf{x},t)\mathbf{G}(\mathbf{x},t)^\mathsf{T}] + \mathbf{G}(\mathbf{x},t)\mathbf{G}(\mathbf{x},t)^\mathsf{T}\nabla_\mathbf{x}\log p_t(\mathbf{x})\Big]p_t(\mathbf{x})\Big\} \\
&\triangleq -\sum_{i=1}^{d} \frac{\partial}{\partial x_i}[\tilde{f}_i(\mathbf{x},t)p_t(\mathbf{x})],
\end{aligned}
$$

做时间逆转

$$
\frac{\partial p_t(\mathbf{x})}{\partial t} = -\sum_{i=1}^{d} \frac{\partial}{\partial x_i}[-\tilde{f}_i(\mathbf{x},t)p_t(\mathbf{x})] \tag{2}
$$

Proof Sketch

整理(2)，得

$$\frac{\partial p_t(\mathbf{x})}{\partial t} = -\sum_{i=1}^{d} \frac{\partial}{\partial x_i}[\bar{f}_i(\mathbf{x},t)p_t(\mathbf{x})] + \frac{1}{2}\sum_{i=1}^{d}\sum_{j=1}^{d}\frac{\partial^2}{\partial x_i \partial x_j}\left[\sum_{k=1}^{d} G_{ik}(\mathbf{x},t)G_{jk}(\mathbf{x},t)p_t(\mathbf{x})\right]$$

其中

$$\bar{\mathbf{f}}(\mathbf{x},t) = \mathbf{f}(\mathbf{x},t) - \nabla \cdot [\mathbf{G}(\mathbf{x},t)\mathbf{G}(\mathbf{x},t)^{\mathsf{T}}] - \mathbf{G}(\mathbf{x},t)\mathbf{G}(\mathbf{x},t)^{\mathsf{T}}\nabla_{\mathbf{x}} \log p_t(\mathbf{x})$$

所以Reverse SDE 为

$$\mathrm{d}\mathbf{x} = \{\mathbf{f}(\mathbf{x},t) - \nabla \cdot [\mathbf{G}(\mathbf{x},t)\mathbf{G}(\mathbf{x},t)^{\mathsf{T}}] - \mathbf{G}(\mathbf{x},t)\mathbf{G}(\mathbf{x},t)^{\mathsf{T}}\nabla_{\mathbf{x}} \log p_t(\mathbf{x})\}\mathrm{d}t + \mathbf{G}(\mathbf{x},t)\mathrm{d}\bar{\mathbf{w}}$$

Forward Process of DDPM & OU Process

考虑离散时间$i = 1, 2, \ldots, N$，DDPM的前向加噪过程

$$\mathbf{x}_i = \sqrt{1-\beta_i}\mathbf{x}_{i-1} + \sqrt{\beta_i}\mathbf{z}_{i-1}, \quad \mathbf{z}_{i-1} \sim \mathcal{N}(0, \mathbf{I}).$$

定义时间步长$\Delta t = \frac{1}{N}$，$t \in \{0, 1, \cdots, \frac{N-1}{N}\}$。加噪schedule为

$$\beta_i = \beta\left(\frac{i}{N}\right) \cdot \frac{1}{N} = \beta(t+\Delta t)\Delta t, \quad N \to \infty, \beta\left(\frac{i}{N}\right) \to \beta(t)$$

于是

$$\begin{aligned}
\mathbf{x}(t+\Delta t) &= \sqrt{1-\beta(t+\Delta t)\Delta t}\mathbf{x}(t) + \sqrt{\beta(t+\Delta t)\Delta t}\mathbf{z}(t) \\
&\approx \mathbf{x}(t) - \frac{1}{2}\beta(t+\Delta t)\Delta t\mathbf{x}(t) + \sqrt{\beta(t+\Delta t)\Delta t}\mathbf{z}(t) \\
&\approx \mathbf{x}(t) - \frac{1}{2}\beta(t)\Delta t\mathbf{x}(t) + \sqrt{\beta(t)\Delta t}\mathbf{z}(t),
\end{aligned}$$

当$\Delta t \to 0$，

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

Denoiser和Score的联系

引理 1 (Tweedie Formula)

对于一个高斯随机变量$\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{z}; \boldsymbol{\mu}_z, \boldsymbol{\Sigma}_z)$，有

$$\mathbb{E}\left[\boldsymbol{\mu}_z | \boldsymbol{z}\right] = \boldsymbol{z} + \boldsymbol{\Sigma}_z \nabla_z \log p(\boldsymbol{z})$$

在DDPM中，我们证明过

$$q(\boldsymbol{x}_t | \boldsymbol{x}_0) = \mathcal{N}(\boldsymbol{x}_t; \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0, (1-\bar{\alpha}_t)\mathbf{I})$$

应用Tweedie Formula

$$\mathbb{E}\left[\boldsymbol{\mu}_{x_t} | \boldsymbol{x}_t\right] = \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 = \boldsymbol{x}_t + (1-\bar{\alpha}_t)\nabla \log p(\boldsymbol{x}_t)$$

带入到$\boldsymbol{\mu}_q(\boldsymbol{x}_t, \boldsymbol{x}_0) = \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})\boldsymbol{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)\boldsymbol{x}_0}{1-\bar{\alpha}_t}$中计算，有

$$\boldsymbol{\mu}_q(\boldsymbol{x}_t, \boldsymbol{x}_0) = \frac{1}{\sqrt{\alpha_t}}\boldsymbol{x}_t + \frac{1-\alpha_t}{\sqrt{\alpha_t}}\nabla \log p(\boldsymbol{x}_t)$$

Denoiser和Score的联系

可以通过学习到的Score计算

$$\mu_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t) = \frac{1}{\sqrt{\alpha_t}}\boldsymbol{x}_t + \frac{1-\alpha_t}{\sqrt{\alpha_t}}\boldsymbol{s}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t)$$

又由

$$\boldsymbol{x}_0 = \frac{\boldsymbol{x}_t + (1-\bar{\alpha}_t)\nabla\log p(\boldsymbol{x}_t)}{\sqrt{\bar{\alpha}_t}} = \frac{\boldsymbol{x}_t - \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_0}{\sqrt{\bar{\alpha}_t}}$$

可以得到Denoiser和Score的联系

$$\nabla\log p(\boldsymbol{x}_t) = -\frac{1}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_0$$

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Reverse OU Process

- Forward process

$$\mathrm{d}\mathbf{X}_t = -\beta_t \mathbf{X}_t \mathrm{d}t + \sqrt{2\beta_t}\mathrm{d}\mathbf{B}_t$$

- Backward process (BP)

$$\mathrm{d}\mathbf{Y}_t = \beta_{T-t}\{\mathbf{Y}_t + 2\nabla \log p_{T-t}(\mathbf{Y}_t)\}\mathrm{d}t + \sqrt{2\beta_{T-t}}\mathrm{d}\mathbf{B}_t$$

Diffusion Model 收敛性分析

- Girsanov 定理
  - Chen S, et al. Sampling is as easy as learning the score: theory for diffusion models with minimal data assumptions. ICLR. 2023.
  - Chen H, et al. Improved analysis of score-based generative modeling: User-friendly bounds under minimal smoothness assumptions. ICML. 2023.
  - Benton J, et al. Nearly d-Linear Convergence Bounds for Diffusion Models via Stochastic Localization. ICLR. 2024
- Log-Sobolev inequality
  - Convergence for score-based generative modeling with polynomial complexity. NeuralPS. 2022.
  - Convergence of score-based generative modeling for general data distributions. 2023.
- 其他
  - A Note on the Convergence of Denoising Diffusion Probabilistic Models. TMLR. 2024.

Reverse Diffusion Monte Carlo[5]

设采样目标为$x \propto e^{-f_*(x)}$，考虑 Reverse Diffusion Process

$$\mathrm{d}\mathbf{X}_t = \beta_{T-t}\{\mathbf{X}_t + 2\nabla \log p_{T-t}(\mathbf{X}_t)\}\mathrm{d}t + \sqrt{2\beta_{T-t}}\mathrm{d}\mathbf{B}_t$$

引理 2

The score function can be rewritten as

$$\nabla_{\boldsymbol{x}} \log p_{T-t}(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{x}_0 \sim q_{T-t}(\cdot|\boldsymbol{x})} \frac{e^{-(T-t)}\boldsymbol{x}_0 - \boldsymbol{x}}{\left(1 - e^{-2(T-t)}\right)},$$

where

$$q_{T-t}(\boldsymbol{x}_0|\boldsymbol{x}) \propto \exp\left(-f_*(\boldsymbol{x}_0) - \frac{\left\|\boldsymbol{x} - e^{-(T-t)}\boldsymbol{x}_0\right\|^2}{2\left(1 - e^{-2(T-t)}\right)}\right).$$

[5]Huang X, Dong H, Yifan H A O, et al. Reverse diffusion monte carlo[C]//The Twelfth International Conference on Learning Representations. 2024.

Reverse Diffusion Monte Carlo

Algorithm 1 RDMC: reverse diffusion Monte Carlo

Input: Initial particle $\tilde{\boldsymbol{x}}_0$ sampled from $\tilde{p}_0$, Terminal time T, Step size η, η', Sample size n.
for $k = 0$ to $\lfloor T/\eta \rfloor - 1$ **do**
  Set $\boldsymbol{v}_k = \boldsymbol{0}$;
  Create n Monte Carlo samples to estimate
  $$\boldsymbol{v}_k \approx \mathbb{E}_{\boldsymbol{x} \sim q_{T-t}} \left[-\frac{\tilde{\boldsymbol{x}}_{k\eta} - e^{-(T-k\eta)}\boldsymbol{x}}{\left(1 - e^{-2(T-k\eta)}\right)} \right], \text{ where } q_{T-t}(\boldsymbol{x}|\tilde{\boldsymbol{x}}_{k\eta}) \propto \exp\left(-f_*(\boldsymbol{x}) - \frac{\left\| \tilde{\boldsymbol{x}}_{k\eta} - e^{-(T-k\eta)}\boldsymbol{x} \right\|^2}{2\left(1 - e^{-2(T-k\eta)}\right)} \right).$$
  $\tilde{\boldsymbol{x}}_{(k+1)\eta} = e^{\eta} \tilde{\boldsymbol{x}}_{k\eta} + (e^{\eta} - 1)\, \boldsymbol{v}_k + \xi$ where ξ is sampled from $\mathcal{N}\left(0, \left(e^{2\eta} - 1\right) \boldsymbol{I}_d\right)$.
end for
Return: $\tilde{\boldsymbol{x}}_{\lfloor T/\eta \rfloor \eta}$.

Thanks & Questions