SDE

参考：生成扩散模型漫谈（五）：一般框架之SDE篇 - 科学空间|Scientific Spaces

前向SDE

前向过程由下述方程给出

$$\mathrm{d}\boldsymbol{x} = f_t(\boldsymbol{x}_t)\mathrm{d}t + g_t \mathrm{d}\boldsymbol{w} \tag{1}$$

以一定精度(Δt 越小越精确)离散化

$$\boldsymbol{x}_{t+\Delta t} - \boldsymbol{x}_t = f_t(\boldsymbol{x}_t)\Delta t + g_t\sqrt{\Delta t}\boldsymbol{\epsilon} \tag{2}$$

SDE(1)提供了对扩散模型进行理论分析的手段，我们借助微分方程对模型进行分析，实际应用时则借助离散的数值方法(2)来求解

逆向SDE

(2)等价于

$$\begin{aligned} p(\boldsymbol{x}_{t+\Delta t}|\boldsymbol{x}_t) &= \mathcal{N}(\boldsymbol{x}_t + f_t(\boldsymbol{x}_t)\Delta t, g_t^2\Delta t\mathbf{I}) \\ &\propto \exp\left(-\frac{\|\boldsymbol{x}_{t+\Delta t} - \boldsymbol{x}_t - f_t(\boldsymbol{x}_t)\Delta t\|^2}{2g_t^2\Delta t}\right) \end{aligned}$$

我们要求解逆向SDE等价于求解$p(\boldsymbol{x}_t|\boldsymbol{x}_{t+\Delta t})$

$$\begin{aligned} p(\boldsymbol{x}_t|\boldsymbol{x}_{t+\Delta t}) &= \frac{p(\boldsymbol{x}_{t+\Delta t}|\boldsymbol{x}_t)p(\boldsymbol{x}_t)}{p(\boldsymbol{x}_{t+\Delta t})} \\ &\propto \exp\left(-\frac{\|\boldsymbol{x}_{t+\Delta t} - \boldsymbol{x}_t - f_t(\boldsymbol{x}_t)\Delta t\|^2}{2g_t^2\Delta t} + \log p(\boldsymbol{x}_t) - \log p(\boldsymbol{x}_{t+\Delta t})\right) \end{aligned}$$

当$\Delta t \to 0$时，上述分布退化为Dirac分布，也就是说，在$\boldsymbol{x}_t$足够靠近$\boldsymbol{x}_{t+\Delta t}$时上述概率明显非0(其余数据点在极限意义下没有考虑必要，高阶余项在极限下为0)，因此只需考虑$\boldsymbol{x}_t$的邻域内一阶展开

$$\log p(\boldsymbol{x}_{t+\Delta t}) = \log p(\boldsymbol{x}_t) + (\boldsymbol{x}_{t+\Delta t} - \boldsymbol{x}_t)\nabla_{\boldsymbol{x}_t}\log p(\boldsymbol{x}_t) + \Delta t\frac{\partial}{\partial t}\log p(\boldsymbol{x}_t)$$

回代入上式并配方有

$$
\begin{aligned}
p(\boldsymbol{x}_t|\boldsymbol{x}_{t+\Delta t}) &\propto \exp\left(-\frac{\|\boldsymbol{x}_{t+\Delta t}-\boldsymbol{x}_t-f_t(\boldsymbol{x}_t)\Delta t\|^2}{2g_t^2\Delta t}-(\boldsymbol{x}_{t+\Delta t}-\boldsymbol{x}_t)\nabla_{\boldsymbol{x}_t}\log p(\boldsymbol{x}_t)+\mathcal{O}(\Delta t)\right)\\
&\propto \exp\left(-\frac{\|\boldsymbol{x}_{t+\Delta t}-\boldsymbol{x}_t-f_t(\boldsymbol{x}_t)\Delta t\|^2+2g_t^2\Delta t(\boldsymbol{x}_{t+\Delta t}-\boldsymbol{x}_t)\cdot\nabla_{\boldsymbol{x}_t}\log p(\boldsymbol{x}_t)}{2g_t^2\Delta t}+\mathcal{O}(\Delta t)\right)\\
&\propto \exp\left(-\frac{\|\boldsymbol{x}_{t+\Delta t}-\boldsymbol{x}_t-\Delta t[f_t(\boldsymbol{x}_t)-g_t^2\nabla_{\boldsymbol{x}_t}\log p(\boldsymbol{x}_t)]\|^2}{2g_t^2\Delta t}+\mathcal{O}(\Delta t)\right)
\end{aligned}
$$

令$\Delta t\to 0$，有

$$
\begin{aligned}
p(\boldsymbol{x}_t|\boldsymbol{x}_{t+\Delta t}) &\propto \exp\left(-\frac{\|\boldsymbol{x}_{t+\Delta t}-\boldsymbol{x}_t-\Delta t[f_t(\boldsymbol{x}_t)-g_t^2\nabla_{\boldsymbol{x}_t}\log p(\boldsymbol{x}_t)]\|^2}{2g_t^2\Delta t}\right)\\
&\approx \exp\left(-\frac{\|\boldsymbol{x}_t-\boldsymbol{x}_{t+\Delta t}+\Delta t[f_{t+\Delta t}(\boldsymbol{x}_{t+\Delta t})-g_{t+\Delta t}^2\nabla_{\boldsymbol{x}_{t+\Delta t}}\log p(\boldsymbol{x}_{t+\Delta t})]\|^2}{2g_{t+\Delta t}^2\Delta t}\right)
\end{aligned}
$$

因此

$$
p(\boldsymbol{x}_t|\boldsymbol{x}_{t+\Delta t})\approx\mathcal{N}(\boldsymbol{x}_{t+\Delta t}+\Delta t[f_{t+\Delta t}(\boldsymbol{x}_{t+\Delta t})-g_{t+\Delta t}^2\nabla_{\boldsymbol{x}_{t+\Delta t}}\log p(\boldsymbol{x}_{t+\Delta t})],g_{t+\Delta t}^2\Delta t\mathbf{I})
$$

于是，对应逆向SDE为

$$
\mathrm{d}\boldsymbol{x}=[f_t(\boldsymbol{x}_t)-g_t^2\nabla_{\boldsymbol{x}_t}\log p(\boldsymbol{x}_t)]\mathrm{d}t+g_t\mathrm{d}\boldsymbol{w}
$$

Score Matching

现在我们的目标归结为求得分函数$\nabla_{\boldsymbol{x}_t}\log p(\boldsymbol{x}_t)$

$$
\begin{aligned}
\nabla_{\boldsymbol{x}_t}\log p(\boldsymbol{x}_t) &= \nabla_{\boldsymbol{x}_t}\log\mathbb{E}_{\boldsymbol{x}_0}\log p(\boldsymbol{x}_t|\boldsymbol{x}_0)\\
&=\frac{\nabla_{\boldsymbol{x}_t}\mathbb{E}_{\boldsymbol{x}_0}\log p(\boldsymbol{x}_t|\boldsymbol{x}_0)}{\mathbb{E}_{\boldsymbol{x}_0}\log p(\boldsymbol{x}_t|\boldsymbol{x}_0)}\\
&=\frac{\mathbb{E}_{\boldsymbol{x}_0}[p(\boldsymbol{x}_t|\boldsymbol{x}_0)\nabla_{\boldsymbol{x}_t}\log p(\boldsymbol{x}_t|\boldsymbol{x}_0)]}{\mathbb{E}_{\boldsymbol{x}_0}\log p(\boldsymbol{x}_t|\boldsymbol{x}_0)}
\end{aligned}
$$

为了得到最终的Loss函数，先给出引理

> Lemma 1. $\arg\min_\mu\mathbb{E}_{\boldsymbol{x}}[g(\boldsymbol{x})\|\mu-f(\boldsymbol{x})\|^2]=\frac{\mathbb{E}_{\boldsymbol{x}}[g(\boldsymbol{x})f(\boldsymbol{x})]}{\mathbb{E}_{\boldsymbol{x}}g(\boldsymbol{x})}$

引理的证明是显然的

因此，我们有

$$
\nabla_{\boldsymbol{x}_t}\log p(\boldsymbol{x}_t)=\arg\min_\mu\mathbb{E}_{\boldsymbol{x}_0}[p(\boldsymbol{x}_t|\boldsymbol{x}_0)\|\mu-\nabla_{\boldsymbol{x}_t}\log p(\boldsymbol{x}_t|\boldsymbol{x}_0)\|^2]
$$

又由于我们对所有$\boldsymbol{x}_t$都要最小化，因此最终的Loss为上面代价函数的积分

$$
\int_{\boldsymbol{x}_t}\mathbb{E}_{\boldsymbol{x}_0}[p(\boldsymbol{x}_t|\boldsymbol{x}_0)\|\mu-\nabla_{\boldsymbol{x}_t}\log p(\boldsymbol{x}_t|\boldsymbol{x}_0)\|^2]\mathrm{d}\boldsymbol{x}_t=\mathbb{E}_{\boldsymbol{x}_0,\boldsymbol{x}_t\sim p(\boldsymbol{x}_t|\boldsymbol{x}_0)}\|\mu-\nabla_{\boldsymbol{x}_t}\log p(\boldsymbol{x}_t|\boldsymbol{x}_0)\|^2
$$

用$s_\theta(\boldsymbol{x}_t,t)$拟合条件得分

$$\mathcal{L}=\mathbb{E}_{\boldsymbol{x}_0,\boldsymbol{x}_t\sim p(\boldsymbol{x}_t|\boldsymbol{x}_0)}\|s_\theta(\boldsymbol{x}_t,t)-\nabla_{\boldsymbol{x}_t}\log p(\boldsymbol{x}_t|\boldsymbol{x}_0)\|^2$$

至此，DDPM最终的Loss推导完毕

Note: 这里原参考的证明可能不是很严谨，我在这里给出相对严谨的证明

从条件路径反推SDE

从SDE求解条件路径$p(\boldsymbol{x}_t|\boldsymbol{x}_0)$涉及SDE的闭式求解，往往困难，反之则相对容易

我们先定义

$$p(\boldsymbol{x}_t|\boldsymbol{x}_0)=\mathcal{N}(\bar{\alpha}_t\boldsymbol{x}_0,\bar{\beta}_t^2\mathbf{I})$$

下面推导对应的SDE

考虑线性解

$$\mathrm{d}\boldsymbol{x}=f_t\boldsymbol{x}\mathrm{d}t+g_t\mathrm{d}\boldsymbol{w}$$

注意到

$$\begin{aligned}\boldsymbol{x}_{t+\Delta t}&=\bar{\alpha}_{t+\Delta t}\boldsymbol{x}_0+\bar{\beta}_{t+\Delta t}\boldsymbol{\epsilon}\\\boldsymbol{x}_t&=\bar{\alpha}_t\boldsymbol{x}_0+\bar{\beta}_t\boldsymbol{\epsilon}_1\\\boldsymbol{x}_{t+\Delta t}&=\boldsymbol{x}_t+f_t\boldsymbol{x}_t\Delta t+g_t\sqrt{\Delta t}\boldsymbol{\epsilon}_2\end{aligned}$$

于是有

$$\begin{aligned}\boldsymbol{x}_{t+\Delta t}&=\boldsymbol{x}_t+f_t\boldsymbol{x}_t\Delta t+g_t\sqrt{\Delta t}\boldsymbol{\epsilon}_2\\&=(1+f_t\Delta t)\boldsymbol{x}_t+g_t\sqrt{\Delta t}\boldsymbol{\epsilon}_2\\&=(1+f_t\Delta t)(\bar{\alpha}_t\boldsymbol{x}_0+\bar{\beta}_t\boldsymbol{\epsilon}_1)+g_t\sqrt{\Delta t}\boldsymbol{\epsilon}_2\\&=\bar{\alpha}_t(1+f_t\Delta t)\boldsymbol{x}_0+[\bar{\beta}_t(1+f_t\Delta t)\boldsymbol{\epsilon}_1+g_t\sqrt{\Delta t}\boldsymbol{\epsilon}_2]\\&=\bar{\alpha}_{t+\Delta t}\boldsymbol{x}_0+\bar{\beta}_{t+\Delta t}\boldsymbol{\epsilon}\end{aligned}$$

对比最后两行，可得

$$\begin{aligned}\bar{\alpha}_{t+\Delta t}&=\bar{\alpha}_t(1+f_t\Delta t)\\\bar{\beta}_{t+\Delta t}^2&=\bar{\beta}_t^2(1+f_t\Delta t)^2+g_t^2\Delta t\end{aligned}$$

进而有

$$\begin{aligned}\frac{\mathrm{d}\bar{\alpha}_t}{\bar{\alpha}_t}&=f_t\mathrm{d}t\\\mathrm{d}\ln\bar{\alpha}_t&=f_t\mathrm{d}t\\f_t&=\frac{1}{\bar{\alpha}_t}\frac{\mathrm{d}\bar{\alpha}_t}{\mathrm{d}t}\end{aligned}$$

代入下方的式子有

$$
\begin{aligned}
g_t^2 \mathrm{d}t &= \bar{\beta}_{t+\mathrm{d}t}^2 - \bar{\beta}_t^2 (1 + f_t \mathrm{d}t)^2 \\
g_t^2 &= \frac{\mathrm{d}\bar{\beta}_t^2}{\mathrm{d}t} - 2\bar{\beta}_t^2 f_t \\
&= 2\frac{\mathrm{d}\bar{\beta}_t}{\mathrm{d}t} - 2\frac{\bar{\beta}_t^2}{\bar{\alpha}_t}\frac{\mathrm{d}\bar{\alpha}_t}{\mathrm{d}t} \\
&= 2\bar{\alpha}_t\bar{\beta}_t\left(\frac{1}{\bar{\alpha}_t}\frac{\mathrm{d}\bar{\beta}_t}{\mathrm{d}t} - \frac{\bar{\beta}_t}{\bar{\alpha}_t^2}\frac{\mathrm{d}\bar{\alpha}_t}{\mathrm{d}t}\right) \\
&= 2\bar{\alpha}_t\bar{\beta}_t\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\bar{\beta}_t}{\bar{\alpha}_t}\right)
\end{aligned}
$$

于是得到对应的SDE

$$
\begin{aligned}
\mathrm{d}\boldsymbol{x} &= f_t \boldsymbol{x} \mathrm{d}t + g_t \mathrm{d}\boldsymbol{w} \\
f_t &= \frac{1}{\bar{\alpha}_t}\frac{\mathrm{d}\bar{\alpha}_t}{\mathrm{d}t} \\
g_t^2 &= 2\bar{\alpha}_t\bar{\beta}_t\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\bar{\beta}_t}{\bar{\alpha}_t}\right)
\end{aligned}
$$

若取$\bar{\alpha}_t \equiv 1$，即为Variance Exploding SDE；$\bar{\alpha}_t^2 + \bar{\beta}_t^2 = 1$时为Variance Preserving SDE

此时

$$
\nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{x}_t|\boldsymbol{x}_0) = -\frac{\boldsymbol{x}_t - \bar{\alpha}_t\boldsymbol{x}_0}{\bar{\beta}_t^2} = -\frac{\boldsymbol{\epsilon}}{\bar{\beta}_t}
$$

令

$$
s_\theta(\boldsymbol{x}_t, t) = -\frac{\boldsymbol{\epsilon}_\theta(\boldsymbol{x}_t, t)}{\bar{\beta}_t}
$$

则有Loss

$$
\mathcal{L} = \frac{1}{\bar{\beta}_t^2}\mathbb{E}_{\boldsymbol{x}_0\sim p(\boldsymbol{x}_0), \boldsymbol{\epsilon}\sim\mathcal{N}(\mathbf{0},\mathbf{I})}\|\boldsymbol{\epsilon}_\theta(\bar{\alpha}_t\boldsymbol{x}_0 + \bar{\beta}_t\boldsymbol{\epsilon}, t) - \boldsymbol{\epsilon}\|^2
$$