

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

逆向SDE

Score Matching

从条件路径反推SDE

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

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

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<mark>离散的数</mark>值方法(2)来求解

逆向SDE

(2)等价于

$$egin{aligned} p(oldsymbol{x}_{t+\Delta t}|oldsymbol{x}_t) &= \mathcal{N}(oldsymbol{x}_t + f_t(oldsymbol{x}_t)\Delta t, g_t^2 \Delta t \mathbf{I}) \ &\propto \exp\left(-rac{\|oldsymbol{x}_{t+\Delta t} - oldsymbol{x}_t - f_t(oldsymbol{x}_t)\Delta t\|^2}{2g_t^2 \Delta t}
ight) \end{aligned}$$

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

$$egin{aligned} p(oldsymbol{x}_t | oldsymbol{x}_{t+\Delta t}) &= rac{p(oldsymbol{x}_{t+\Delta t} | oldsymbol{x}_t) p(oldsymbol{x}_t)}{p(oldsymbol{x}_{t+\Delta t})} \ &\propto \exp\left(-rac{\|oldsymbol{x}_{t+\Delta t} - oldsymbol{x}_t - f_t(oldsymbol{x}_t) \Delta t\|^2}{2g_t^2 \Delta t} + \log p(oldsymbol{x}_t) - \log p(oldsymbol{x}_{t+\Delta t})
ight) \end{aligned}$$

当 $\Delta t \to 0$ 时,上述分布退化为Dirac分布,也就是说,在 $m{x}_t$ 足够靠近 $m{x}_{t+\Delta t}$ 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 $m{x}_t$ 的邻域内一阶展开

$$\log p(oldsymbol{x}_{t+\Delta t}) = \log p(oldsymbol{x}_t) + (oldsymbol{x}_{t+\Delta t} - oldsymbol{x}_t)
abla_{oldsymbol{x}_t} \log p(oldsymbol{x}_t) + \Delta t rac{\partial}{\partial t} \log p(oldsymbol{x}_t)$$

回代入上式并配方有

$$egin{aligned} p(oldsymbol{x}_t | oldsymbol{x}_{t+\Delta t}) &\propto \exp\left(-rac{\|oldsymbol{x}_{t+\Delta t} - oldsymbol{x}_t - f_t(oldsymbol{x}_t)\Delta t\|^2}{2g_t^2 \Delta t} - (oldsymbol{x}_{t+\Delta t} - oldsymbol{x}_t)
abla_{oldsymbol{x}_t} \log p(oldsymbol{x}_t) + \mathcal{O}(\Delta t)
ight) \ &\propto \exp\left(-rac{\|oldsymbol{x}_{t+\Delta t} - oldsymbol{x}_t - f_t(oldsymbol{x}_t)\Delta t\|^2 + 2g_t^2 \Delta t(oldsymbol{x}_{t+\Delta t} - oldsymbol{x}_t) \cdot
abla_{oldsymbol{x}_t} \log p(oldsymbol{x}_t)}{2g_t^2 \Delta t} + \mathcal{O}(\Delta t)
ight) \ &\propto \exp\left(-rac{\|oldsymbol{x}_{t+\Delta t} - oldsymbol{x}_t - \Delta t[f_t(oldsymbol{x}_t) - g_t^2
abla_{oldsymbol{x}_t} \log p(oldsymbol{x}_t)]\|^2}{2g_t^2 \Delta t} + \mathcal{O}(\Delta t)
ight) \end{aligned}$$

$$egin{aligned} p(oldsymbol{x}_t | oldsymbol{x}_{t+\Delta t}) & \propto \exp\left(-rac{\|oldsymbol{x}_{t+\Delta t} - oldsymbol{x}_t - \Delta t[f_t(oldsymbol{x}_t) - g_t^2
abla_{oldsymbol{x}_t} \log p(oldsymbol{x}_t)]\|^2}{2g_t^2 \Delta t}
ight) \ & pprox \exp\left(-rac{\|oldsymbol{x}_{t+\Delta t} + \Delta t[f_{t+\Delta t}(oldsymbol{x}_{t+\Delta t}) - g_{t+\Delta t}^2
abla_{oldsymbol{x}_{t+\Delta t}} \log p(oldsymbol{x}_{t+\Delta t})]\|^2}{2g_{t+\Delta t}^2 \Delta t}
ight) \end{aligned}$$

因此

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

于是,对应逆向SDE为

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

Score Matching

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

$$egin{aligned}
abla_{oldsymbol{x}_t} \log p(oldsymbol{x}_t) &=
abla_{oldsymbol{x}_t} \log \mathbb{E}_{oldsymbol{x}_0} \log p(oldsymbol{x}_t | oldsymbol{x}_0) \ &= rac{
abla_{oldsymbol{x}_t} \mathbb{E}_{oldsymbol{x}_0} \log p(oldsymbol{x}_t | oldsymbol{x}_0)}{\mathbb{E}_{oldsymbol{x}_0} [p(oldsymbol{x}_t | oldsymbol{x}_0)
abla_{oldsymbol{x}_t} \log p(oldsymbol{x}_t | oldsymbol{x}_0)]} \ &= rac{\mathbb{E}_{oldsymbol{x}_0} [p(oldsymbol{x}_t | oldsymbol{x}_0)
abla_{oldsymbol{x}_t} \log p(oldsymbol{x}_t | oldsymbol{x}_0)]}{\mathbb{E}_{oldsymbol{x}_t} \log p(oldsymbol{x}_t | oldsymbol{x}_0)} \end{aligned}$$

为了得到最终的Loss函数、先给出引理

Lemma 1.
$$rg\min_{\mu}\mathbb{E}_{m{x}}[g(m{x})\|\mu-f(m{x})\|^2]=rac{\mathbb{E}_{m{x}}[g(m{x})f(m{x})]}{\mathbb{E}_{m{x}}g(m{x})}$$

引理的证明是显然的

因此, 我们有

$$abla_{oldsymbol{x}_t} \log p(oldsymbol{x}_t) = rg \min_{\mu} \mathbb{E}_{oldsymbol{x}_0}[p(oldsymbol{x}_t | oldsymbol{x}_0) \| \mu -
abla_{oldsymbol{x}_t} \log p(oldsymbol{x}_t | oldsymbol{x}_0) \|^2]$$

又由于我们对所有 x_t 都要最小化,因此最终的Loss为上面代价函数的积分

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

用 $s_{\theta}(\boldsymbol{x}_{t},t)$ 拟合条件得分

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

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

$$p(oldsymbol{x}_t|oldsymbol{x}_0) = \mathcal{N}(ar{lpha}_toldsymbol{x}_0,ar{eta}_t^2oldsymbol{ ext{I}})$$

下面推导对应的SDE

考虑线性解

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

注意到

$$egin{aligned} oldsymbol{x}_{t+\Delta t} &= ar{lpha}_{t+\Delta t} oldsymbol{x}_0 + ar{eta}_{t+\Delta t} oldsymbol{\epsilon} \ oldsymbol{x}_t &= ar{lpha}_t oldsymbol{x}_0 + ar{eta}_t oldsymbol{\epsilon}_1 \ oldsymbol{x}_{t+\Delta t} &= oldsymbol{x}_t + f_t oldsymbol{x}_t \Delta t + g_t \sqrt{\Delta t} oldsymbol{\epsilon}_2 \end{aligned}$$

于是有

$$egin{aligned} oldsymbol{x}_{t+\Delta t} &= oldsymbol{x}_t + f_t oldsymbol{x}_t \Delta t + g_t \sqrt{\Delta t} oldsymbol{\epsilon}_2 \ &= (1 + f_t \Delta t) oldsymbol{x}_t + g_t \sqrt{\Delta t} oldsymbol{\epsilon}_2 \ &= (1 + f_t \Delta t) (ar{lpha}_t oldsymbol{x}_0 + ar{eta}_t oldsymbol{\epsilon}_1) + g_t \sqrt{\Delta t} oldsymbol{\epsilon}_2 \ &= ar{lpha}_t (1 + f_t \Delta t) oldsymbol{x}_0 + [ar{eta}_t (1 + f_t \Delta t) oldsymbol{\epsilon}_1 + g_t \sqrt{\Delta t} oldsymbol{\epsilon}_2] \ &= ar{lpha}_{t+\Delta t} oldsymbol{x}_0 + ar{eta}_{t+\Delta t} oldsymbol{\epsilon} \end{aligned}$$

对比最后两行, 可得

$$egin{aligned} ar{lpha}_{t+\Delta t} &= ar{lpha}_t (1 + f_t \Delta t) \ ar{eta}_{t+\Delta t}^2 &= ar{eta}_t^2 (1 + f_t \Delta t)^2 + g_t^2 \Delta t \end{aligned}$$

进而有

$$egin{aligned} rac{\mathrm{d}ar{lpha}_t}{ar{lpha}_t} &= f_t \mathrm{d}t \ \mathrm{d}\lnar{lpha}_t &= f_t \mathrm{d}t \end{aligned} \ f_t &= rac{1}{ar{lpha}_t} rac{\mathrm{d}ar{lpha}_t}{\mathrm{d}t}$$

代入下方的式子有

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

于是得到对应的SDE

$$egin{align} \mathrm{d}oldsymbol{x} &= f_toldsymbol{x}\mathrm{d}t + g_t\mathrm{d}oldsymbol{w} \ f_t &= rac{1}{ar{lpha}_t}rac{\mathrm{d}ar{lpha}_t}{\mathrm{d}t} \ g_t^2 &= 2ar{lpha}_tar{eta}_trac{\mathrm{d}}{\mathrm{d}t}\left(rac{ar{eta}_t}{ar{lpha}_t}
ight) \end{aligned}$$

若取 $arlpha_t\equiv 1$,即为Variance Exploding SDE; $arlpha_t^2+areta_t^2=1$ 时为Variance Preserving SDE

此时

$$abla_{oldsymbol{x}_t} \log p(oldsymbol{x}_t | oldsymbol{x}_0) = -rac{oldsymbol{x}_t - ar{lpha}_t oldsymbol{x}_0}{ar{eta}_t^2} = -rac{oldsymbol{\epsilon}}{ar{eta}_t}$$

令

$$s_{ heta}(oldsymbol{x}_t,t) = -rac{oldsymbol{\epsilon}_{ heta}(oldsymbol{x}_t,t)}{ar{eta}_t}$$

则有Loss

$$\mathcal{L} = rac{1}{ar{eta}_t^2} \mathbb{E}_{m{x}_0 \sim p(m{x}_0), m{\epsilon} \sim \mathcal{N}(m{0}, m{I})} \|m{\epsilon}_{ heta}(ar{lpha}_t m{x}_0 + ar{eta}_t m{\epsilon}, t) - m{\epsilon}\|^2$$