条件扩散模型

扩散后验采样

图片 $x_0 \longleftrightarrow x_T$ 白噪音

$q_t(x_t \mid y) = \int q_t(x_t\ x_0 \mid y)\, dx_0$

$= \int q_0(x_t \mid x_0)\, q_t(x_0 \mid y)$

目标：采样 $q_0(x_0 \mid y)$

$X_0 \sim q_0(X_0 \mid y)$

$dX_t = f(t) X_t\, dt + g(t)\, dW_t$ $\qquad X_t \sim q_t(x_t \mid y)$

计算 $\nabla_x \log q_{T-t}(x \mid y)$

$$= \nabla_x \log \frac{q_{T-t}(y \mid x)\, q_{T-t}(x)}{q(y)}$$

$$= \nabla_x \log q_{T-t}(y \mid x)\, q_{T-t}(x)$$

$$= \nabla_x \log q_{T-t}(y \mid x) + \nabla_x \log \underbrace{q_{T-t}(x)}_{\text{score}}$$

$$q_t(y \mid x) = \int q_t(y\ x_0 \mid x)\, dx_0$$

$$= \int q_t(y \mid x_0\ x)\, q_t(x_0 \mid x)\, dx_0$$

$$= \int \underbrace{q_0(y \mid x_0)}_{\text{似然函数}}\, \underbrace{q_{t0}(x_0 \mid x)}_{\text{计算}}\, dx_0$$

Tweedie 公式

$$q_{0t}(x_t \mid x_0) = N(x_t \mid \lambda_t x_0, \sigma_t^2 I)$$

$$q_{t0}(x_0 \mid x_t) = \frac{q_{0t}(x_t \mid x_0)\, q_0(x_0)}{q_t(x_t)}$$

$$e^{-\frac{1}{2}\frac{(x-\lambda_t x_0)^2}{\sigma_t^2}}$$

$$q_t(x_t) = \int q_{0t}(x_t \mid x_0)\, q_0(x_0)\, dx_0$$

$$\nabla q_t(x_t) = \int q_{0t}(x_t \mid x_0) \left(-\frac{x_t - \lambda_t x_0}{\sigma_t^2}\right) q_0(x_0)\, dx_0$$

$$\frac{\nabla q_t(x_t)}{q_t(x_t)} = \int q_{0t}(x_0 \mid x_t) \left(-\frac{x_t - \lambda_t x_0}{\sigma_t^2}\right) dx_0$$

$$= -\frac{x_t}{\sigma_t^2} + \frac{\lambda_t}{\sigma_t^2} E_{q_{t0}(x_0 \mid x_t)}\, x_0$$

$$E_{q_{t0}(x_0 \mid x_t)}\, x_0 = \frac{x_t}{\lambda_t} + \frac{\sigma_t^2}{\lambda_t} \nabla \log q_t(x_t)$$

Twisted 扩散采样

$$q(x_{0:T}|y) = \frac{q(x_{0:T}, y)}{q(y)} = \frac{q(y|x_{0:T})\, q(x_{0:T})}{q(y)}$$

$$= \frac{q(y|x_0)\, q_T(x_T) \prod_{t=0}^{T-1} q_{t+1,t}(x_t | x_{t+1})}{q(y)}$$

似然函数

如果有 $X_T\ X_{T-1} \cdots X_0$，满足这个条件分布，

那么 $X_0 \sim q_0(x_0 | y)$

重要性采样

$X_T \sim q_T(x_T)$

$X_t | X_{t+1} \sim q_{t+1,t}(x_t | x_{t+1}) \quad t = T-1, T-2, \cdots 2, 1$

扩散模型

$q_{t+1,t}(x_t | x_{t+1}) = N(x_t | m_{t+1|t}, \sigma^2_{t+1|t})$

比如 OU 过程 $\quad X_t = Y_{T-t}$

$$dY_t = [Y_t + 2s_\theta(t, Y_t)]dt + \sqrt{2}\, dW_t$$

$$dX_t = -[X_t + 2s_\theta(t, X_t)]dt + \sqrt{2}\, dW_t \quad (dt = -1)$$

+ 权重

$$m_{t+1|t} = x_{t+1} + (x_{t+1} + 2s_\theta(t, x_{t+1})) \qquad \sigma^2_{t+1|t} = 2$$

最后权重 $w_{0:T} \propto q(y | x_0)$

联合分布满足 $q(x_{0:T} | y)$

序贯蒙特卡洛

$$q(x_{0:T} \mid y) = q(x_T \mid y) \prod_{t=0}^{T-1} q(x_t \mid x_{t+1}, y)$$

$$q(x_T \mid y) \propto q_T(y \mid x_T)\, q_T(x_T)$$

$$q(x_t \mid x_{t+1}, y) = \frac{q_t(y \mid x_t, \cancel{x_{t+1}})\, q_{t+1|t}(x_t \mid x_{t+1})}{q_{t+1}(y \mid x_{t+1})}$$

$$q_{t+1|t}(x \mid x_{t+1}) \approx N(x_t \mid m_{t+1|t}, \sigma^2_{t+1|t})$$

比如 OU 过程 $\qquad X_t = Y_{T-t}$

$$dY_t = [Y_t + 2S_\theta(t, Y_t)]dt + \sqrt{2}\, dW_t$$

$$dX_t = -[X_t + 2S_\theta(t, X_t)]dt + \sqrt{2}\, dW_t \qquad (dt = -1)$$

$$m_{t+1|t} = x_{t+1} + (x_{t+1} + 2S_\theta(t, x_{t+1})) \qquad \sigma^2_{t+1|t} = 2$$

$$q_0(y \mid \hat{x}_0(t+1, x)) \underset{\sim}{\propto} e^{-\frac{1}{2}\frac{\|x-m\|^2}{\sigma^2_{t+1|t}}}$$

$$m = x_{t+1} + \nabla_x \log q_0(y \mid \hat{x}_0(t+1, x_{t+1})) \cdot \sigma^2_{t+1|t}$$

$$m + m_{t+1|t} = x_{t+1} + 2(x_{t+1} + S_\theta(t, x_{t+1})$$
$$+ \nabla_x \log q_0)$$

渐近精确

$$q_T(x_T)\cdot q_0(y\,|\,\hat{x}_0(T, x_T))\prod_{t=0}^{T-1}\tilde{q}_{t+1\,t}(x_t\,|\,x_{t+1}, y)\,w_t$$

$$= q_T(x_T)\,q_0(y\,|\,\hat{x}_0(T, x_T))\prod_{t=0}^{T-1}\frac{q_0(y\,|\,\hat{x}_0(t, x_t))\,q_{t+1\,t}(x_t\,|\,x_{t+1})}{q_0(y\,|\,\hat{x}_0(t+1, x_{t+1}))}$$

$$= q_T(x_T)\cdot\underbrace{q_0(y\,|\,\hat{x}_0(0, x_0))}_{q_0(y\,|\,x_0)}\prod_{t=0}^{T-1}q_{t+1\,t}(x_t\,|\,x_{t+1})$$

SMC Diffusion Sampler

考虑 方差爆炸 SDE

$$dX_t = \sigma dW_t$$

$$X_t = X_0 + \sqrt{\sigma^2 t}\, W$$

前向方程

$$\partial_t q_t(x) = \frac{\sigma^2}{2} \Delta q_t(x)$$

后向方程

$$\partial_t \rho_t(x) = -\frac{\sigma^2}{2} \Delta \rho_t(x) \qquad \rho_t = q_{T-t}$$

粒子方程

$$dY_t = \sigma^2 \nabla_x \log \rho_t(x)\, dt + \sigma dW_t$$

$$= \sigma^2 \nabla_x \log q_{T-t}(x)\, dt + \sigma dW_t \quad (0 \to T)$$

$$dX_t = -\sigma^2 \nabla_x \log q_t(x)\, dt - \sigma dW_t \quad (T \to 0)$$

$$(dt = -1)$$

$$X_{t-1} = X_t + \sigma^2 \nabla_x \log q_t(X_t) + \sigma dW_1$$

$$\sim N(x_{t-1} \mid X_t + \sigma^2 \nabla_x \log q_t(X_t),\ \sigma^2)$$

Tweedie 公式

$$q_t(y \mid x) \simeq q_0(y \mid \hat{x}_0(t, x))$$

$$E_{q_{t0}(x_0|x)}\, x_0 = \hat{x}_0(t, x)$$

$$\nabla q_t(x) = \nabla \int q(x_0\, x)\, dx_0$$

$$= \int \nabla q_{0t}(x \mid x_0)\, q(x_0)\, dx_0$$

$$= \int q_{0t}(x \mid x_0)\, \frac{-(x - x_0)}{\sigma^2 t}\, q(x_0)\, dx_0$$

$$\frac{\nabla q_t(x)}{q_t(x)} = \int q_{t0}(x_0 \mid x)\, \frac{x_0 - x}{\sigma^2 t}\, dx_0$$

$$\hat{x}_0(t, x) = \sigma^2 t\, \nabla \log q_t(x) + x$$

proposal

$$q_0(y \mid \hat{x}_0(t, x))\, q_{t+1\,t}(x \mid x_{t+1})$$

$$p_\eta(y - G(x - \sigma^2 t S_\theta(t, x))) \qquad N(\sigma^2 S_\theta(t, x_{t+1}), \sigma^2)$$

$$\approx e^{-\frac{1}{2}\frac{\|x - m\|^2}{\sigma^2}} \qquad e^{-\frac{1}{2}\frac{\|x - \tilde{m}\|^2}{\sigma^2}}$$

$$\tilde{m} = \sigma^2 S_\theta(t, x_{t+1})$$

$$m \approx x_{t+1} + \sigma^2 \nabla_x \log p_\eta(x_{t+1})$$

$$m + \tilde{m} = x_{t+1} + \sigma^2 \left(\nabla_x \log p_\eta(x_{t+1}) + S_\theta(t, x_{t+1})\right)$$

$$C = \sigma^2$$