

条件扩散模型 (CONDITIONED DIFFUSION MODEL)

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条件生成模型

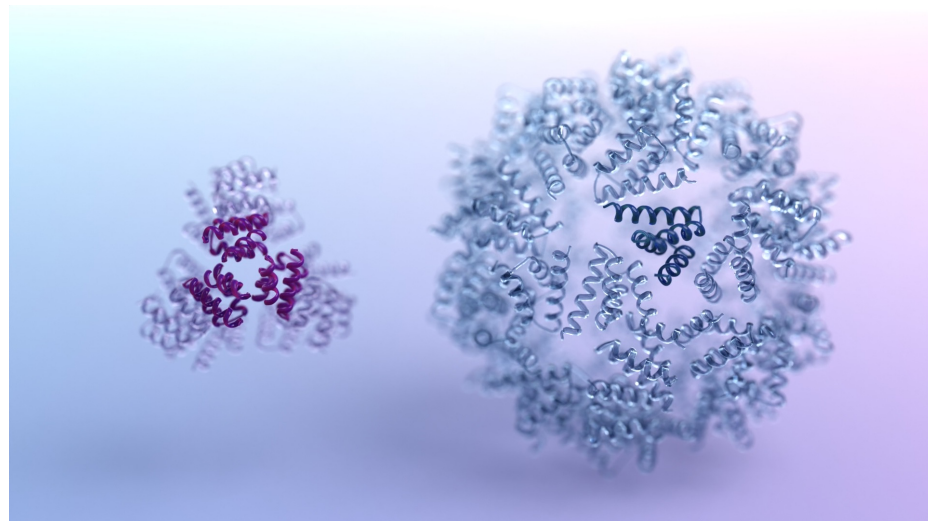
➤ 应用：图像修复、去噪，蛋白质设计



Before inpainting



After inpainting





条件生成模型

➤ 扩散模型

$$q_0(x) \approx \frac{1}{N} \sum_i \delta(x - x^{*i})$$

生成 $x \sim q_0(x)$

➤ 条件扩散模型

已知似然函数 $q_0(y|x)$

目标：在扩散模型的基础上， $s_\theta(t, x) \approx \nabla \log q_{T-t}(x)$

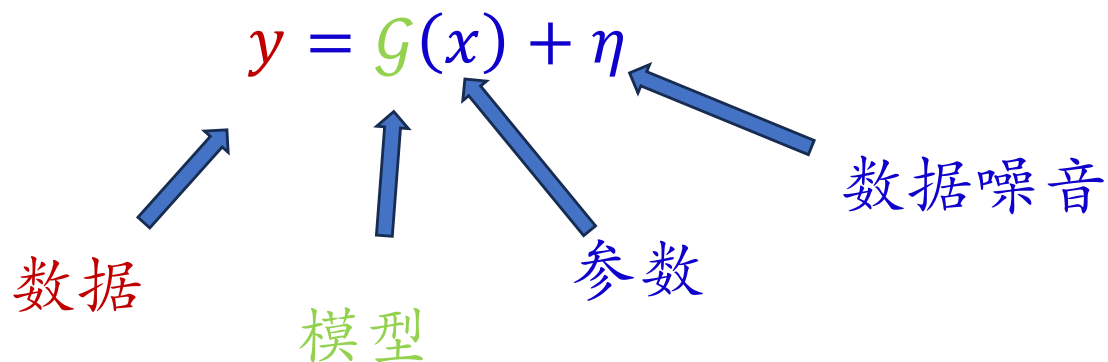
生成 $x \sim q_0(x|y) \propto q_0(y|x)q_0(x)$

注： q_t 在不同上下文中具有不同含义



条件生成模型

➤ 贝叶斯反问题



$$\text{后验分布: } q_0(x|y) \propto q_0(y|x)q_0(x)$$

$$\text{似然函数: } q_0(y|x) = \rho_\eta(y - G(x))$$

➤ 之前设置

$$q_0(x) = e^{-\Phi_0(x)}$$

新设置

$$q_0(x) \approx \frac{1}{N} \sum_i \delta(x - x^{*i})$$



条件生成模型

➤ 扩散后验采样 (diffusion posterior sampling)

假设 $X_0 \sim q_0(x)$ ，我们有前向和后向过程

$$dX_t = f(t)X_t dt + g(t)dW_t \quad (0 \rightarrow T, \text{图片} \rightarrow \text{白噪音})$$

$$dY_t = \hat{f}(t, Y_t)dt + \hat{g}(t)dW_t \quad (0 \rightarrow T, \text{白噪音} \rightarrow \text{图片})$$

我们有条件

$$y = G(x) + \eta$$

且给定 X_0 ， X_t 和 y 相互独立。按照贝叶斯观点，我们可以考虑 X_t ， y 的条件概率 $q_t(x|y)$ ，我们的目标是采样

$$q_0(x|y)$$



梯度诱导扩散模型

➤ 扩散后验采样(diffusion posterior sampling)

假设 $X_0 \sim q_0(x_0|y)$ ，直接使用生成模型

$$dX_t = f(t)X_t dt + g(t)dW_t$$

那么 $X_t \sim q_t(x_t|y) \propto q_t(y|x_t)q_t(x_t)$

OU后向过程条件生成

$$\partial_t \rho_t(x|y) = -\nabla \cdot [(x + \nabla \log q_{T-t}(x|y)) \rho_t(x|y)]$$

贝叶斯法则

$$\nabla \log q_{T-t}(x|y) = \nabla \log q_{T-t}(y|x) + \nabla \log q_{T-t}(x)$$

梯度诱导项

分数函数



梯度诱导扩散模型

➤ Tweedie 公式近似

似然函数

$$\begin{aligned}\nabla \log q_t(y|x) &= \nabla \log \int q_{t0}(x_0|x) q_0(y|x_0) dx_0 \\ &\approx \nabla \log q_0(y|\hat{x}_0(t, x))\end{aligned}$$

其中

$$q_{0t}(x|x_0) = \mathcal{N}(x; \lambda_t x_0, \sigma_t^2 I)$$

做如下近似

$$q_{t0}(x_0|x) \approx \delta(x_0 - \hat{x}_0(t, x))$$

$$\hat{x}_0(t, x) = \mathbb{E}_{q_{t0}(x_0|x)}[x_0] = \frac{1}{\lambda_t} (x + \sigma_t^2 \nabla \log q_t(x))$$

➤ 诱导导数计算

$$\nabla \log q_{T-t}(y|\hat{x}_0(T-t, x)) = \nabla_x \log \rho_\eta(y - \mathcal{G}(\hat{x}_0(T-t, x)))$$



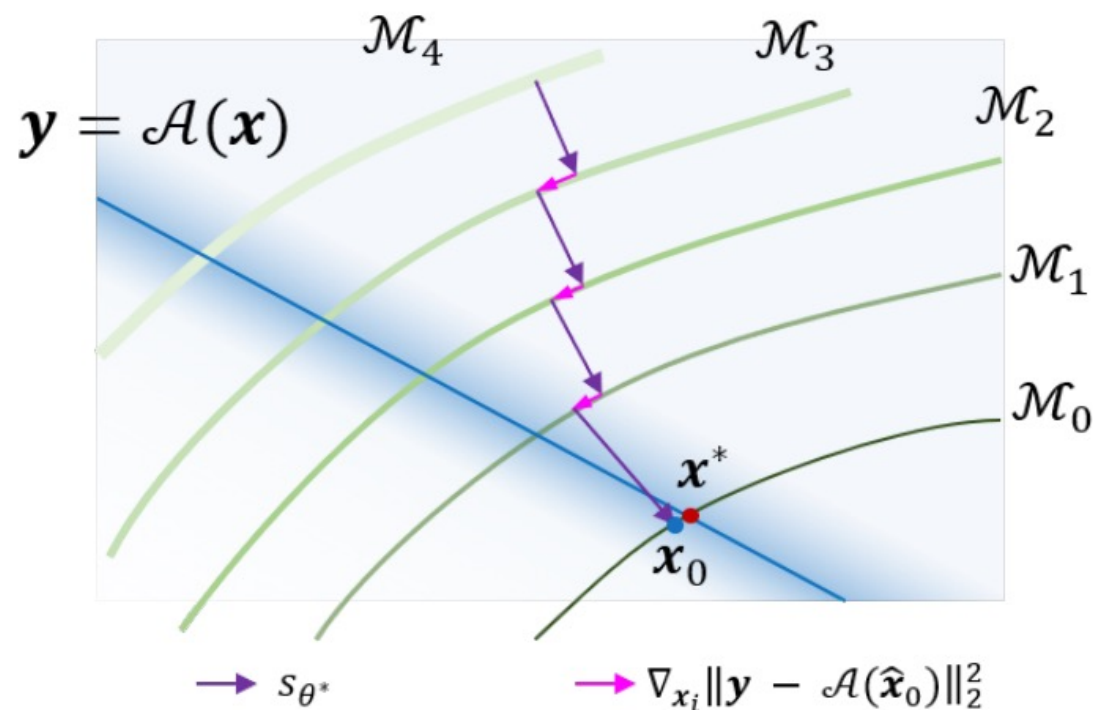
梯度诱导扩散模型

➤ 扩散后验采样

后向过程条件生成 ($0 \rightarrow T$)

$$\partial_t \rho_t(x|y)$$

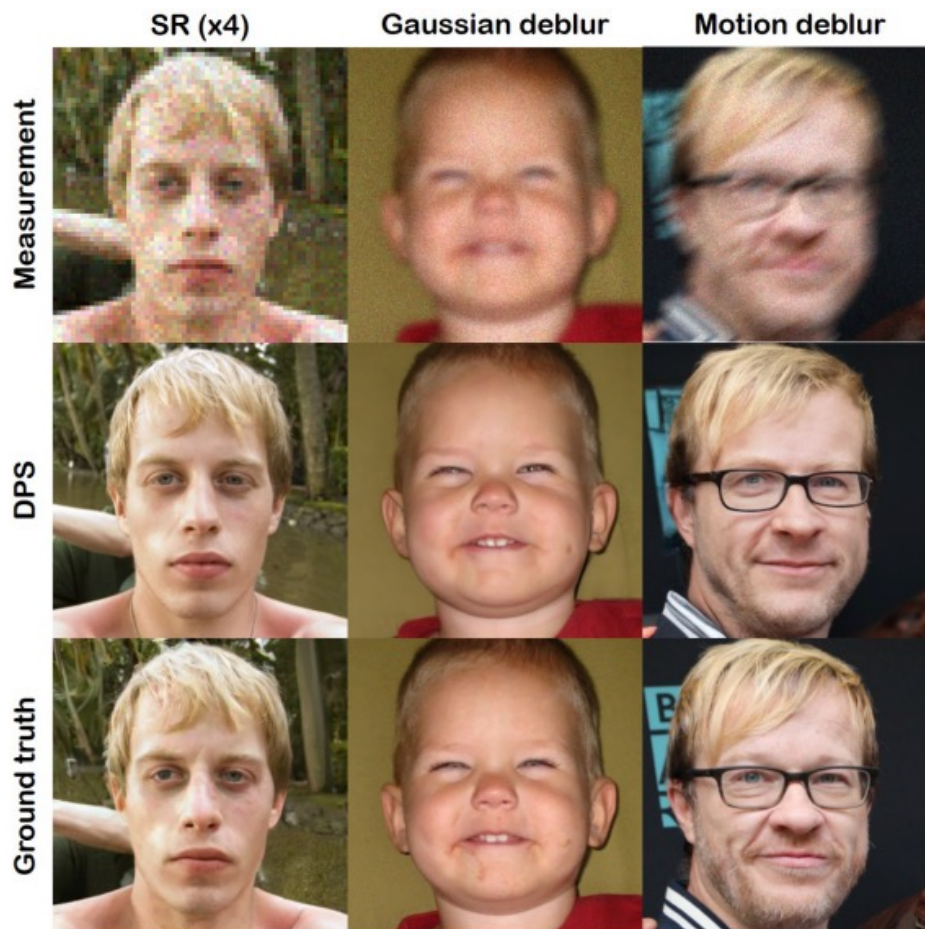
$$= -\nabla \cdot [(x + \nabla \log q_{T-t}(x) + \nabla \log q_0(y|\hat{x}_0(T-t, x))) \rho_t(x|y)]$$





梯度诱导扩散模型

➤ 扩散后验采样



能不能修正
Tweedie 公式
近似的误差，
达到渐近精确
(asymptotically
exact) ?

权重修正！

Chung, Hyungjin, et al. "Diffusion posterior sampling for general noisy inverse problems." *arXiv preprint arXiv:2209.14687* (2022)



序贯蒙特卡洛扩散模型

➤ 扩散后验采样(diffusion posterior sampling)

假设 $X_0 \sim q_0(x)$ ，我们有前向和后向过程

$$dX_t = f(t)X_t dt + g(t)dW_t \quad (0 \rightarrow T, \text{图片} \rightarrow \text{白噪音})$$

$$dY_t = \hat{f}(t, Y_t)dt + \hat{g}(t)dW_t \quad (0 \rightarrow T, \text{白噪音} \rightarrow \text{图片})$$

我们有条件

$$y = \mathcal{G}(x) + \eta$$

考虑时间离散($t = 0, 1, \dots, T$)的条件分布

$$q(x_{0:T}|y) = \frac{q_0(y|x_0)q_T(x_T) \prod_{t=0}^{T-1} q_{t+1t}(x_t|x_{t+1})}{q(y)}$$



序贯蒙特卡洛扩散模型

➤ 重要性采样

考虑时间离散($t = 0, 1, \dots, T$)的条件分布

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

扩散模型

$$X_T \sim q_T(x_T)$$

$$X_t|X_{t+1} \sim q_{t+1t}(x_t|X_{t+1}) \approx \mathcal{N}(x_t|m_{t+1|t}, \sigma_{t+1|t}^2)$$

$t = T - 1, \dots, 0$

OU过程： $m_{t+1|t} = X_{t+1} + (X_{t+1} + 2s_\theta(t+1, X_{t+1}))$,

$$\sigma_{t+1|t}^2 = 2$$

计算权重

权重退化为0！ $w(X_{0:T}) \propto q(y|X_0)$



序贯蒙特卡洛扩散模型

➤ 最优 (optimal) 序贯蒙特卡洛

考虑时间离散 ($t = 0, 1, \dots, T$) 的条件分布

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

采样

$$X_T \sim q_T(x_T|y) \propto q_T(y|x_T)q_T(x_T)$$

$$\begin{aligned} X_t|X_{t+1} \sim q_{t+1t}(x_t|X_{t+1}, y) \propto q_t(y|x_t)q_{t+1t}(x_t|X_{t+1}) \\ t = T - 1, \dots, 0 \end{aligned}$$

不需要权重！



序贯蒙特卡洛扩散模型

➤ Tweedie 公式近似

似然函数

$$q_t(y|x) \propto \int q_{t0}(x_0|x)q_0(y|x_0)dx_0$$
$$\approx q_0(y|\hat{x}_0(t, x))$$

其中

$$q_{0t}(x|x_0) = \mathcal{N}(x; \lambda_t x_0, \sigma_t^2 I)$$

做如下近似

$$q_{t0}(x_0|x) \approx \delta(x_0 - \hat{x}_0(t, x))$$

$$\hat{x}_0(t, x) = \mathbb{E}_{q_{t0}(x_0|x)}[x_0] = \frac{1}{\lambda_t} (x + \sigma_t^2 \nabla \log q_t(x))$$



序贯蒙特卡洛扩散模型

➤ 序贯蒙特卡洛

采样 $j = 1, \dots, J$

$$X_T^j \sim X_T \sim q_T(x_T), \quad w_T^j \propto q_0(y|\hat{x}_0(T, X_T))$$

对于 $t = T - 1, \dots, 0$ (隐去上标 j)

$$X_t|X_{t+1} \sim \tilde{q}_{t+1,t}(x_t|X_{t+1}, y) \approx q_0(y|\hat{x}_0(t+1, x_t))q_{t+1t}(x_t|X_{t+1})$$

高斯提议核 (OU过程):

$$\begin{aligned} &\tilde{q}_{t+1,t}(x|X_{t+1}, y) \\ &\approx \mathcal{N}(x, X_{t+1} + 2(\nabla_x \log q_0(y|\hat{x}_0(t+1, X_{t+1}))) + X_{t+1} + s_\theta(t+1, X_{t+1}), 2) \end{aligned}$$

$$\text{权重: } w_t \propto \frac{q_0(y|\hat{x}_0(t, X_t))q_{t+1t}(X_t|X_{t+1})}{q_0(y|\hat{x}_0(t+1, X_{t+1}))\tilde{q}_{t+1,t}(X_t|X_{t+1}, y)}$$

梯度诱导项

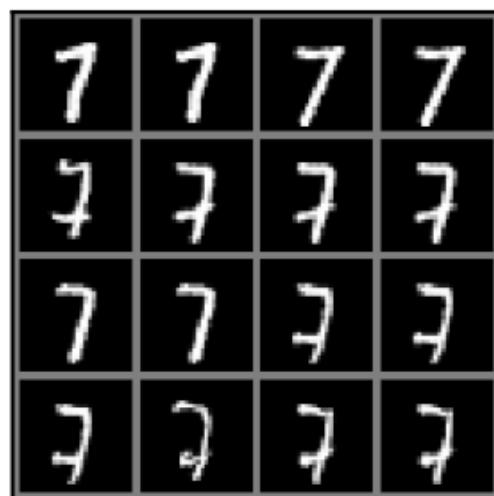
渐近精确:

$$\left\{ X_{0:T}, \prod_{t=0}^{T-1} w_t \right\} \sim q_T(x_T)q_0(y|\hat{x}_0(0, x)) \prod_{t=0}^{T-1} q_{t+1t}(x_t|X_{t+1})$$



序贯蒙特卡洛扩散模型

➤ 序贯蒙特卡洛



TDS



Gradient Guidance

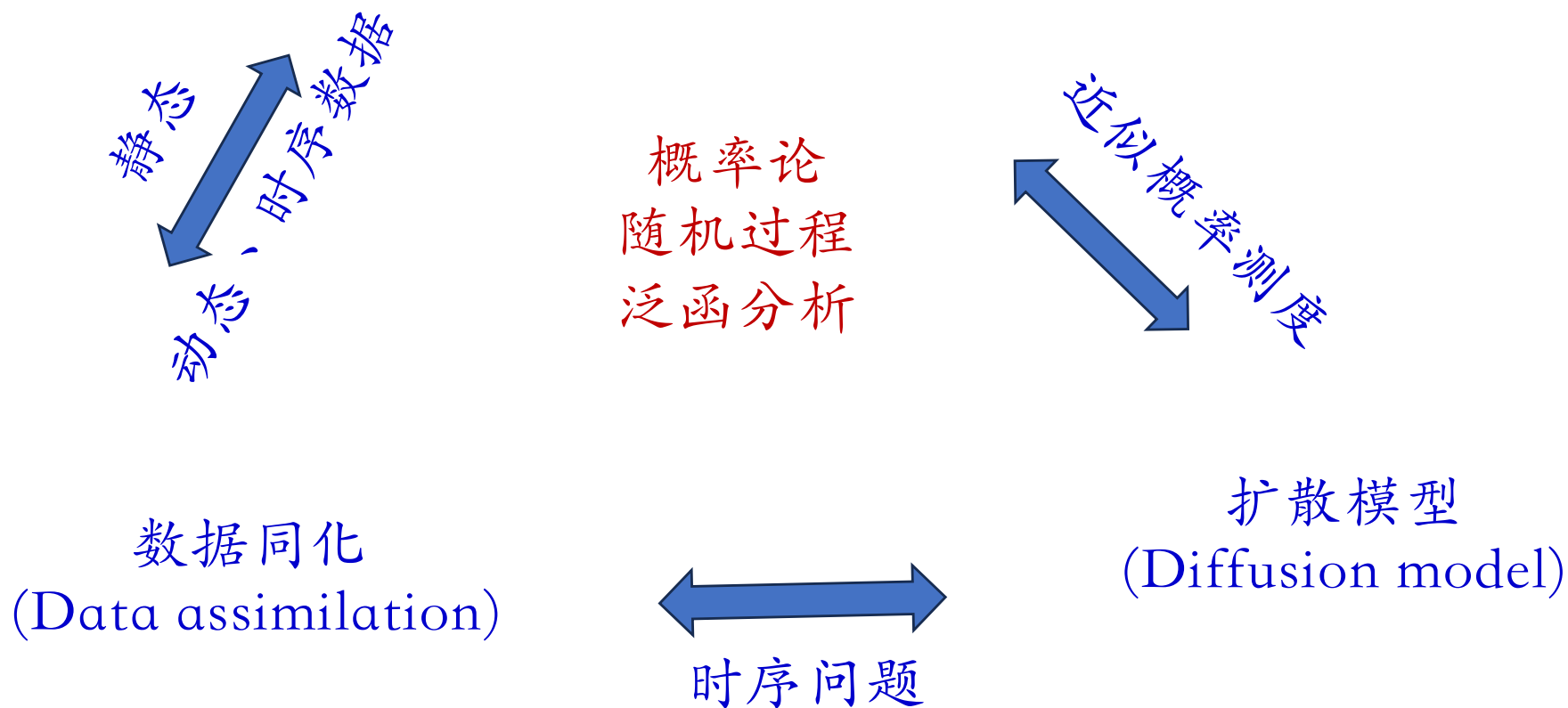
Wu, Luhuan, et al. "Practical and asymptotically exact conditional sampling in diffusion models." *Advances in Neural Information Processing Systems* 36 (2024).



课程回顾

➤ 课程内容回顾

贝叶斯反问题
(Bayesian inverse problems)





扩展阅读

➤ 梯度诱导扩散模型

Chung, Hyungjin, et al. "Diffusion posterior sampling for general noisy inverse problems." *arXiv preprint arXiv:2209.14687* (2022)

➤ 序贯蒙特卡洛扩散模型

Wu, Luhuan, et al. "Practical and asymptotically exact conditional sampling in diffusion models." *Advances in Neural Information Processing Systems* 36 (2024).