扩散模型
(DIFFUSION MODEL)

黄政宇
北京大学北京国际数学研究中心
北京大学国际机器学习研究中心

生成模型

- 应用：视频、音乐生成

生成模型

- 目标分布

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

目标: 采样 $x \sim q_0(x)$

基于分数的生成模型

Forward SDE (data → noise)

$\mathbf{x}(0)$ —— $\mathrm{d}\mathbf{x} = \mathbf{f}(\mathbf{x}, t)\mathrm{d}t + g(t)\mathrm{d}\mathbf{w}$ ——→ $\mathbf{x}(T)$

x^{*i}

score function

$\mathbf{x}(0)$ ←— $\mathrm{d}\mathbf{x} = \left[\mathbf{f}(\mathbf{x}, t) - g^2(t)\nabla_{\mathbf{x}} \log p_t(\mathbf{x})\right] \mathrm{d}t + g(t)\mathrm{d}\bar{\mathbf{w}}$ —— $\mathbf{x}(T)$

Reverse SDE (noise → data)

本堂课大纲

- 扩散过程简介
  - 前向过程
  - 后向过程
    - 去噪扩散概率模型 (denoising diffusion probabilistic model, DDPM)
    - 概率流常微分方程 (probability flow ODE)
- 分数匹配 (score matching)
  - U-Net：分数表示 (score representation)
- 理论分析
- 数值实验
  - 混合高斯模型
  - 手写数字识别 (MNIST)

扩散过程

- 前向过程 $(0 \to T$，图片 → 白噪音)

随机常微分方程 (stochastic differential equation, SDE)：

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

分布：$X_t = \lambda_t X_0 + \sigma_t W, \quad W \sim \mathcal{N}(0, I)$

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

其中

$$f(t) = \frac{d\log\lambda_t}{dt} \qquad g(t)^2 = \frac{d\sigma_t^2}{dt} - 2\frac{d\log\lambda_t}{dt}\sigma_t^2$$

证明思路: 考虑 $L(t,x) = \frac{x}{\lambda_t}$ $dL(t,x_t)$

扩散过程

- 前向过程 $(0 \to T$，图片 $\to$ 白噪音$)$

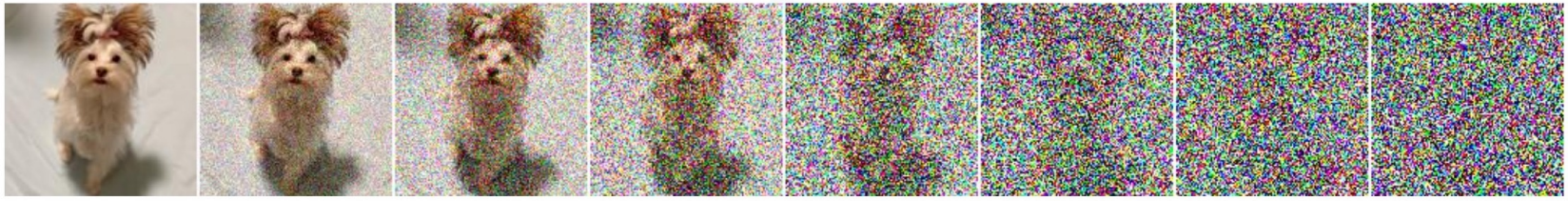
随机常微分方程：

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

密度函数： $X_t \sim q_t(x)$

满足Fokker Planck方程：

$$\partial_t q_t(x) = -\nabla \cdot (f(t)xq_t(x)) + \frac{1}{2}\Delta(g(t)^2 q_t(x))$$



扩散过程

- 反向过程 ($T \to 0$，白噪音 → 图片)

$$-\partial_t q_{T-t}(x) = -\nabla \cdot (f(T-t)x q_{T-t}) + \frac{1}{2}\Delta(g(T-t)^2 q_{T-t})$$

定义：$\rho_t(x) = q_{T-t}(x)$ $(0 \to T)$，满足

$$\partial_t \rho_t(x) = \nabla \cdot (f(T-t)x\rho_t) - \frac{1}{2}\Delta(g(T-t)^2 \rho_t)$$

- 粒子动力学 $(0 \to T)$

生成白噪音：$Y_0 \sim \rho_0(x) = q_T(x)$ $(0 \to T)$

求解：$dY_t = \hat{f}(t, Y_t)dt + \hat{g}(t)dW_t$

前向过程

- Ornstein-Uhlenbeck (OU) 过程 $(0 \to T)$

$$dX_t = -\frac{1}{2}\beta(t)X_t dt + \sqrt{\beta(t)}dW_t$$

$$dX_t = -X_t dt + \sqrt{2}dW_t$$

- 方差爆炸 (Variance exploding) SDE动力学 $(0 \to T)$

$$dX_t = \sigma(t)dW_t$$

$$dX_t = dW_t$$

OU 过程

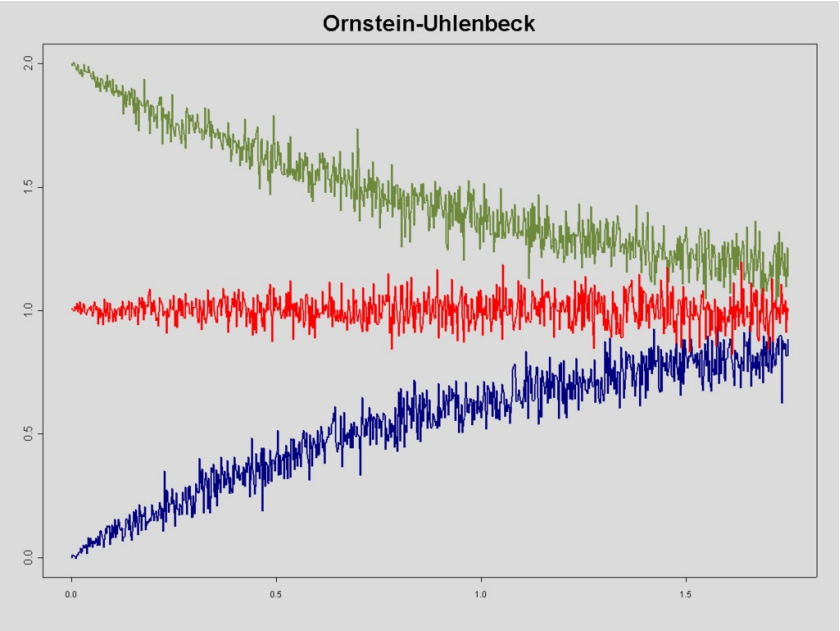
- 前向方程 $(0 \to T)$

SDE: $dX_t = -X_t dt + \sqrt{2} dW_t$

$$\lambda_t = e^{-t} \qquad \sigma_t = \sqrt{1 - e^{-2t}}$$

$$X_t = e^{-t} X_0 + \sqrt{1 - e^{-2t}} W$$

$$X_t \to \mathcal{N}(0, I)$$



密度函数： $X_t \sim q_t(x)$

满足Fokker Planck方程：

$$\partial_t q_t(x) = \nabla \cdot \left((x + \nabla \log q_t(x))\, q_t(x) \right)$$

OU过程

- 后向方程 $(T \to 0)$

$$-\partial_t q_{T-t}(x) = \nabla \cdot \left((x + \nabla \log q_{T-t}(x))\, q_{T-t}(x) \right)$$

定义： $\rho_t(x) = q_{T-t}(x) \qquad (0 \to T)$

$$\partial_t \rho_t(x) = -\nabla \cdot \left((x + \nabla \log q_{T-t}(x))\, \rho_t \right)$$

- 粒子动力学 $(0 \to T)$

生成白噪音： $Y_0 \sim \mathcal{N}(0, I) \approx q_T(x) \qquad (0 \to T)$

- 去噪扩散概率模型 (DDPM)

$$dY_t = (Y_t + 2\nabla \log q_{T-t}(Y_t))dt + \sqrt{2} dW_t$$

- 概率流常微分方程 (probability flow ODE)

$$\frac{dY_t}{dt} = Y_t + \nabla \log q_{T-t}(Y_t)$$

基于分数的生成模型

- 基于分数的生成模型

步骤 1： 添加噪声

$$X_t = e^{-t}X_0 + \sqrt{1-e^{-2t}}W \qquad W \sim \mathcal{N}(0, I)$$

步骤 2：分数匹配

$$s_\theta(t, x) \approx \nabla \log q_{T-t}(x)$$

步骤 3：去噪生成

初始化：$\hat{Y}_0 \sim q_T(x) \approx \mathcal{N}(0, I)$

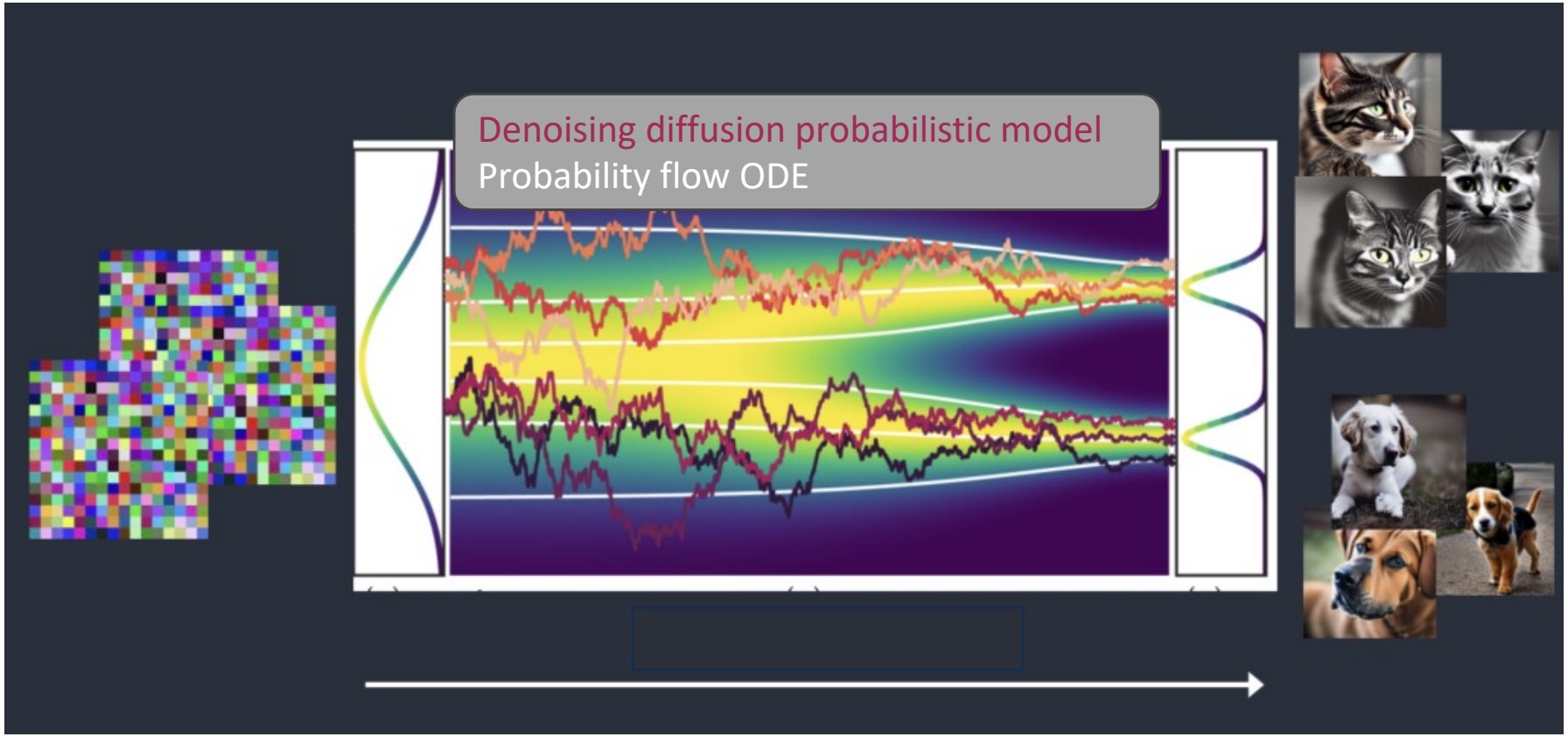
- 去噪扩散概率模型 (DDPM)

$$d\hat{Y}_t = (\hat{Y}_t + 2s_\theta(t, \hat{Y}_t))dt + \sqrt{2}dW_t$$

- 概率流常微分方程 (probability flow ODE)

$$\frac{d\hat{Y}_t}{dt} = \hat{Y}_t + s_\theta(t, \hat{Y}_t)$$

基于分数的生成模型


Denoising diffusion probabilistic model
Probability flow ODE

分数匹配 (Score Matching)

- 目标函数

$$\min_{\theta} \int_0^T w_{T-t} \mathbb{E}_{q_{T-t}} \| s_\theta(t,x) - \nabla \log q_{T-t}(x) \|^2 \, dt$$

数据：

$$X_t = e^{-t} X_0 + \sqrt{1 - e^{-2t}} W \sim q_t(x)$$

概率密度函数：

$$q_{0t}(x|x_0) = \mathcal{N}(x; e^{-t}x_0, (1 - e^{-2t})I)$$

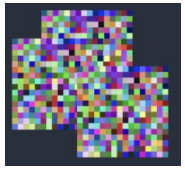
$$q_t(x) = \int \mathcal{N}(x; e^{-t}x_0, (1 - e^{-2t})I) q_0(x_0) dx_0$$

- 数值实现 (Monte Carlo 积分)

$$\min_{\theta} \int_0^T w_{T-t} \mathbb{E}_{q_{0(x_0)}} \mathbb{E}_{q_{0T-t}(x|x_0)} \| s_\theta(t,x) - \nabla \log q_{0T-t}(x|x_0) \|^2$$

分数匹配 (Score Matching)

- 时间离散



$$0 = t_0 < t_1 < \cdots t_N = T - \tau$$

τ: 避免奇异 (singularity)

练习：$q_0 = \delta(x)$， 计算$\nabla \log q_{T-t}(x)$

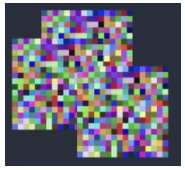
$$q_t(x) = \int \mathcal{N}(x; e^{-t}x_0, (1 - e^{-2t})I) q_0(x_0) dx_0$$

$$= \mathcal{N}(x; 0, (1 - e^{-2t})I)$$

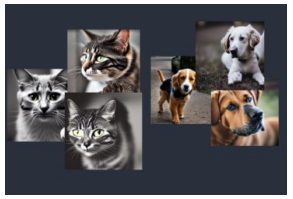
$$s(t,x) = \nabla \log q_{T-t}(x) = -\frac{x}{1-e^{-2(T-t)}} \approx \mathcal{O}\left(\frac{1}{T-t}\right)$$，当 $t \to T$

分数匹配 (Score Matching)

- 时间离散



$$0 = t_0 < t_1 < \cdots t_N = T - \tau$$



$$\min_{\theta} \int_0^{T-\tau} w_{T-t} \mathbb{E}_{q_{0(x_0)}} \mathbb{E}_{q_{0T-t}(x|x_0)} \| s_\theta(t,x) - \nabla \log q_{0T-t}(x|x_0) \|^2$$

- 固定t_i进行训练
- 随机采样t_i进行训练

分数匹配 (Score Matching)

- 估计 $s(x,t) \approx \nabla \log q_{T-t}$

$$\min_{\theta} \int_{\tau}^{T} w_t \mathbb{E}_{q_{0(x_0)}} \mathbb{E}_{q_{0t}(x|x_0)} \| s_\theta(x, T-t) - \nabla \log q_{0t}(x|x_0) \|^2$$

- 权重选取

$$q_t(x|x_0) = \mathcal{N}(x; e^{-t}x_0, (1-e^{-2t})I)$$

$$\nabla \log q_t(x|x_0) = -\frac{x - e^{-t}x_0}{1-e^{-2t}}$$

$$w_t \propto \frac{1}{\mathbb{E}_{q_t(x|x_0)} \|\nabla \log q_t(x|x_0)\|^2} \propto 1 - e^{-2t}$$

- 时间嵌入 (time embedding)

输入： x, $[\sin(2\pi\omega t); \cos(2\pi\omega t)]$

- 噪音预测模型

$$s_\theta(x, T-t) \coloneqq -\epsilon_\theta(x, T-t)/\sqrt{1-e^{-2t}}$$

分数匹配 (Score Matching)

- 噪音预测模型

$$\min_{\theta} \int_{\tau}^{T} w_t \mathbb{E}_{q_{0(x_0)}} \mathbb{E}_{q_{0t}(x|x_0)} \| s_\theta(x, T-t) - \nabla \log q_{0t}(x|x_0) \|^2$$

换元：

$$s_\theta(x, T-t) \coloneqq -\epsilon_\theta(x, T-t)/\sqrt{1-e^{-2t}}$$

目标函数：

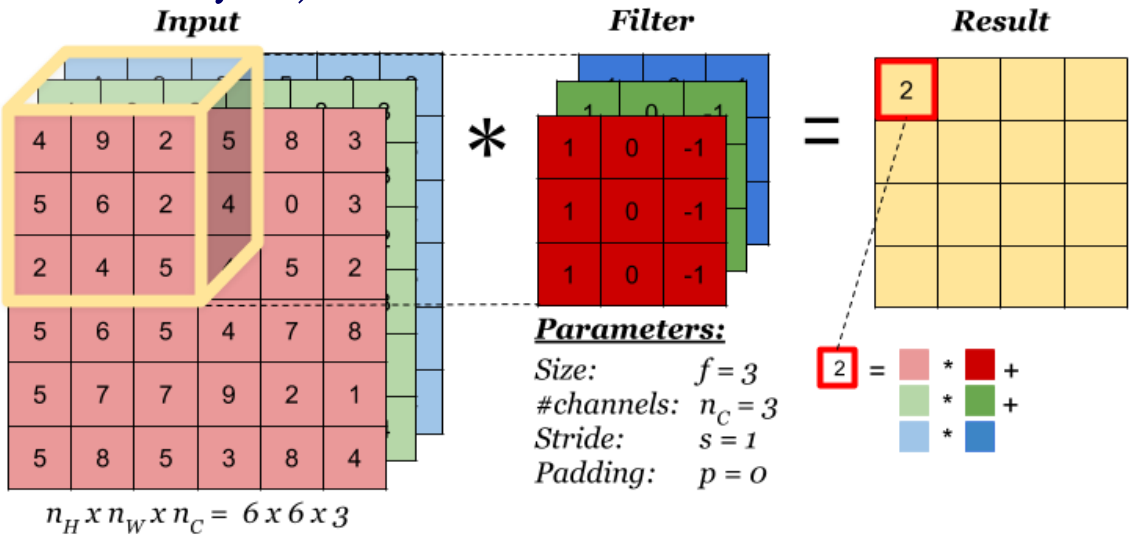
$$\min_{\theta} \int_{\tau}^{T} \frac{w_t}{\sigma_t^2} \mathbb{E}_{q_{0(x_0)}} \mathbb{E}_{x=\lambda_t x_0 + \sigma_t W} \| \epsilon_\theta(x, T-t) - W \|^2$$

其中

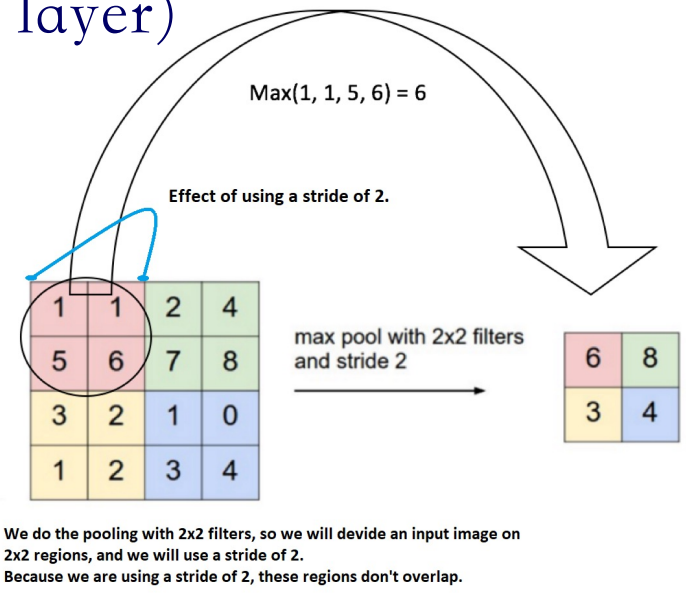
$$\lambda_t = \mathrm{e}^{-t} \qquad w_t \propto \sigma_t^2 = 1 - e^{-2t}$$

U-Net：分数表示$\epsilon_\theta(x,t)$

- 卷积层 (Convolution layer)

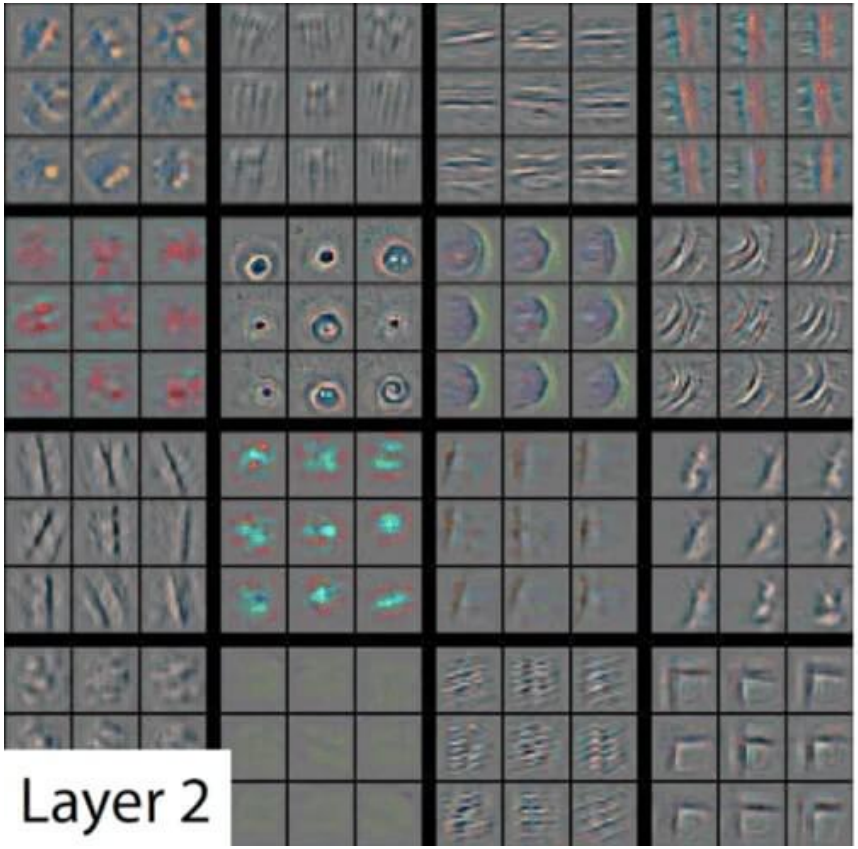


- 池化层 (Pooling layer)



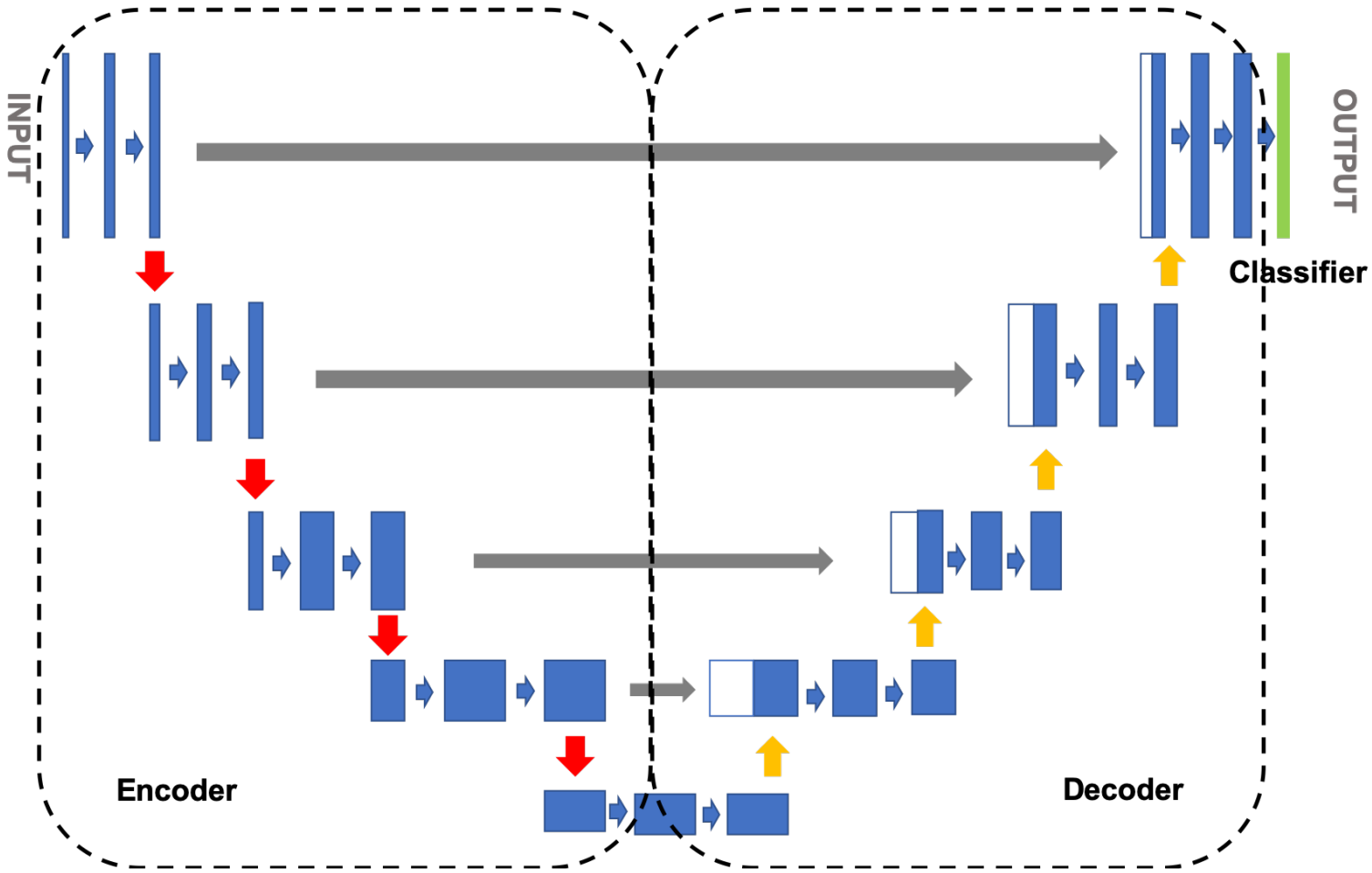
U-Net：分数表示$\epsilon_\theta(x,t)$

- 卷积层 (Convolution layer)

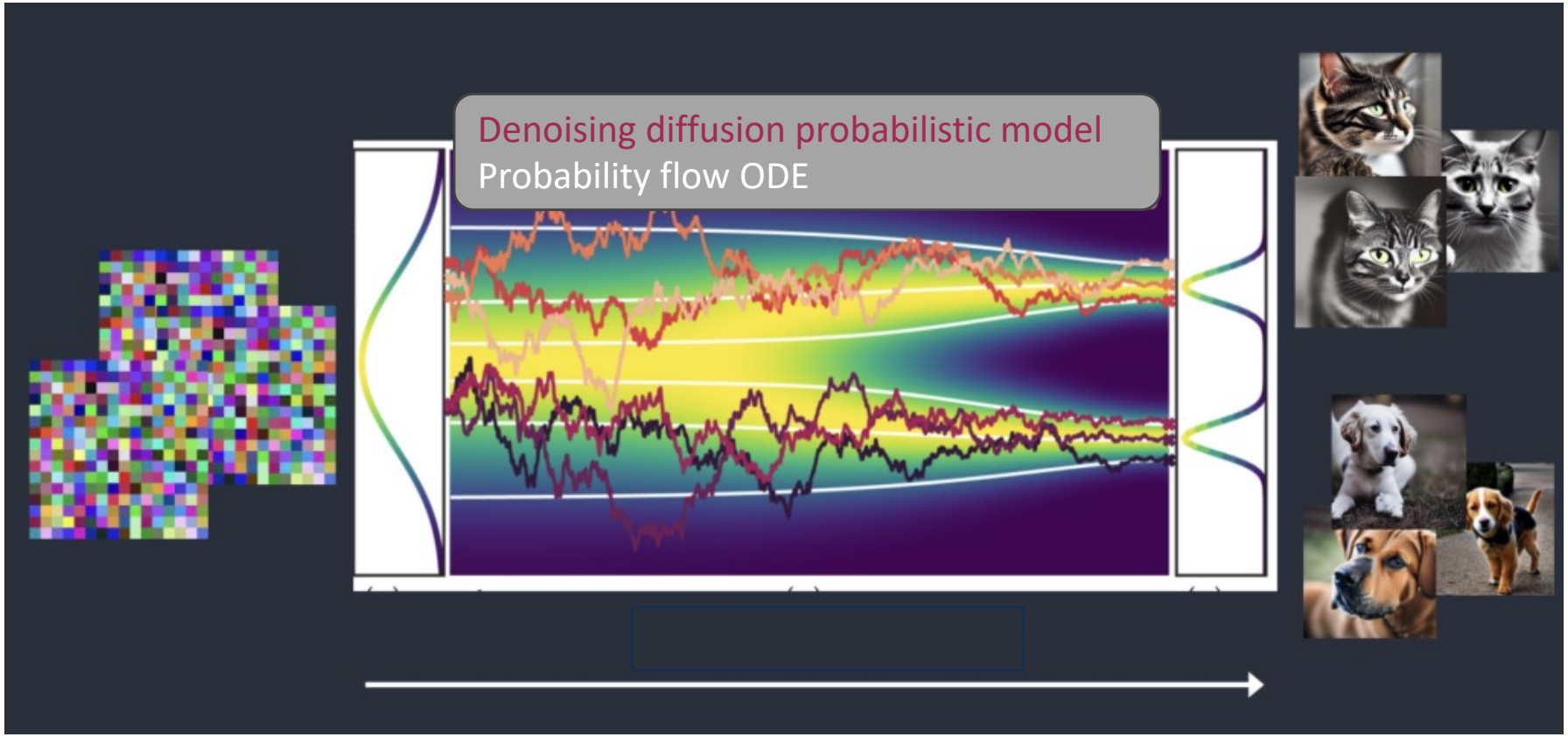


U-Net：分数表示$\epsilon_\theta(x,t)$

- U-Net



基于分数的生成模型


Denoising diffusion probabilistic model
Probability flow ODE

去噪扩散概率模型 (DDPM)

➢ 去噪扩散概率模型

$$d\hat{Y}_t = (\hat{Y}_t + 2s_\theta(t, \hat{Y}_t))\, dt + \sqrt{2}dW_t$$

- Euler-Maruyama

$$d\hat{Y}_t = \left(\hat{Y}_{t_k} + 2s_\theta(t_k, \hat{Y}_{t_k})\right) dt + \sqrt{2}dW_t \qquad t \in [t_k, t_{k+1}]$$

- 指数积分器 (exponential integrator)

$$d\hat{Y}_t = \left(\hat{Y}_t + 2s_\theta(t_k, \hat{Y}_{t_k})\right) dt + \sqrt{2}dW_t \qquad t \in [t_k, t_{k+1}]$$

$\hat{Y}_t \sim \hat{\rho}_t$，$\hat{\rho}_{t_N}$ 和 ρ_T 之间的误差是多少?

$$\partial_t \rho_t(x) = -\nabla \cdot ((x + \nabla \log q_{T-t}(x))\, \rho_t)$$
$$dY_t = \left(Y_t + 2\nabla \log q_{T-t}(Y_t)\right)dt + \sqrt{2}dw_t$$

去噪扩散概率模型 (DDPM)

Girsanov 定理

假设 $y_0 \sim q_T$, 考虑在$C\left([0,T];R^d\right)$ 上的路径测度 Q_T 和 P_T ，它们对应以下两种扩散过程：

$$Q_T: dY_t = \left(Y_t + 2\nabla \log q_{T-t}(Y_t)\right)dt + \sqrt{2}dW_t$$

$$P_T: d\hat{Y}_t = \left(\hat{Y}_t + 2s_\theta\left(t_k, \hat{Y}_{t_k}\right)\right)dt + \sqrt{2}dW_t \quad t \in [t_k, t_{k+1}]$$

$$\mathrm{KL}\left[\rho_{t_N} \parallel \hat{\rho}_{t_N}\right] \leq \mathrm{KL}\left[Q_{t_N} \parallel P_{t_N}\right]$$

$$\leq \sum_{k=0}^{N-1} \int_{t_k}^{t_{k+1}} \mathbb{E}_{Q_{t_N}} \left\| s_\theta\left(t_k, y_{t_k}\right) - \nabla \log q_{T-t}(y_t) \right\|^2 dt$$

去噪扩散概率模型 (DDPM)

误差分析 (Chen el al.2023; Benton el al. 2024)

A1: 分数匹配误差

$$\sum_{k=0}^{N-1}(t_{k+1}-t_k)\mathbb{E}_{q_{t_k}}\left\|s_\theta(t_k,x)-\nabla\log q_{T-t_k}(x)\right\|\le\delta^2$$

A2: 数据假设 $\mathrm{Cov}_{q_0}(x)=I_d$

我们有，当 $0=t_0<t_1\cdots<t_N=T-\tau$, 且 $t_{k+1}-t_k\le\kappa\min\{1,T-t_{k+1}\}$，那么

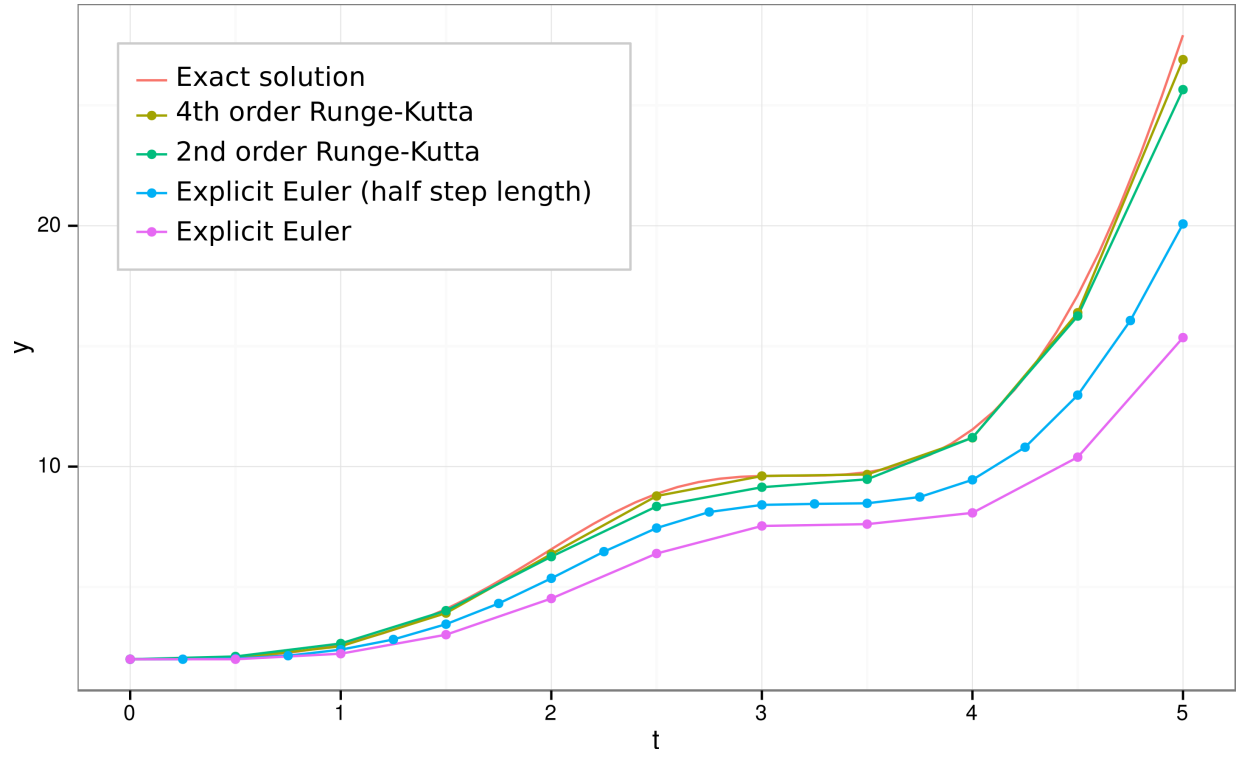
$$KL\left[\rho_T\parallel\hat{\rho}_{t_N}\right]\lesssim\delta^2+d\kappa^2N+\kappa dT+de^{-2T}$$

概率流常微分方程

- 概率流常微分方程 (Probability flow ODE)

$$\frac{d\hat{Y}_t}{dt} = \hat{Y}_t + s_\theta\left(t, \hat{Y}_t\right)$$

高阶格式!
O(10) 个时间步，更高效！



概率流常微分方程

- 概率流常微分方程 (Probability flow ODE)

$$\frac{d\hat{Y}_t}{dt} = \hat{Y}_t + s_\theta\left(t, \hat{Y}\right)$$

- (高阶) Runge-Kutta 格式

$$d\hat{Y}_t = \left(\hat{Y}_{t_k} + s_\theta\left(t_k, \hat{Y}_{t_k}\right)\right) dt \qquad t \in [t_k, t_{k+1}]$$

- (高阶) 指数积分器 (exponential integrator)

$$d\hat{Y}_t = \left(\hat{Y}_t + s_\theta\left(t_k, \hat{Y}_{t_k}\right)\right) dt \qquad t \in [t_k, t_{k+1}]$$

概率流常微分方程

引理 (Huang at el. 2024)

假设 $\rho_t, \hat{\rho}_t \in C^1\left([0,T]; R^d\right) \cap L^1\left([0,T]; R^d\right)$ 是下面两个对流方程的解

$$\partial_t \rho_t(x) = \nabla \cdot (U_t(x)\, \rho_t(x))$$
$$\partial_t \hat{\rho}_t(x) = \nabla \cdot \left(\widehat{U}_t(x) \hat{\rho}_t(x)\right)$$

我们有

$$\left|\mathrm{TV}(\rho_T, \hat{\rho}_T) - \mathrm{TV}(\rho_0, \hat{\rho}_0)\right|$$
$$\leq \frac{1}{2} \int_0^T \int \left|\nabla \cdot \left((U_t(x) - \widehat{U}_t(x))\rho_t(x)\right)\right| dx\, dt$$

概率流常微分方程

假设

A1. 数据有紧支撑$\{x \in R^d : \|x\|_\infty \leq D\}$

A2. 分数匹配误差

$$\int_0^{T-\tau} \mathbb{E}_{q_{T-t}} \|s_\theta(t,x) - \nabla \log q_{T-t}(x)\|^2 dt \leq \delta^2$$

A3.（正则性）$s_\theta(t,x)$ 是 L-Lipschitz连续的。即为了使用 p-th 阶 Runge-Kutta 方法，我们假设$s_\theta(t,x)$前$p+1$ 阶导数被 L约束。

概率流常微分方程

误差分析

如果 $\hat{\rho}_{t_N}$ 是从 $\mathcal{N}(0, I_d)$ 初始化的概率流常微分方程（ODE）的输出。使用 p 阶 Runge-Kutta 方法，均匀步长 $h = \frac{T-\tau}{N}$，得到：

$$\mathrm{TV}(\rho_{t_N}, \hat{\rho}_{t_N}) \leq e^{-T} dD + dT^{\frac{3}{4}}(L + \tau^{-2}D^3)^{\frac{1}{2}}\delta^{\frac{1}{2}} + d(dh)^p(LD)^{p+1}\log\frac{T}{\tau}$$

初始化误差　　得分匹配误差　　离散化误差

- 我们只估计到时间 $T-\tau$ 处的误差，而不是 q_0。q_0 和 $q_\tau = \rho_{t_N}$ 之间的 Wasserstein-2 距离有上界 $\mathcal{O}(\tau + d(\tau D)^2)$
- 理论误差界为 $\mathcal{O}(d\sqrt{\delta} + d(dh)^p)$

数值实验

- 数据分布 q_0

  R^d 中 5-模态的混合高斯

- 得分匹配误差 $(\delta(t,x) = s(t,x) - \nabla \log q_{T-t}(x))$

  1. 常数误差：$\delta(t,x) = \delta \frac{1}{d}$
  2. 线性误差：$\delta(t,x) = \delta \frac{x-m}{d}$
  3. 正弦误差：$\delta(t,x) = \delta \sin x \frac{x-m}{d}$

  其中，m 为高斯混合分布的均值，$\sin x$作用于每个分量

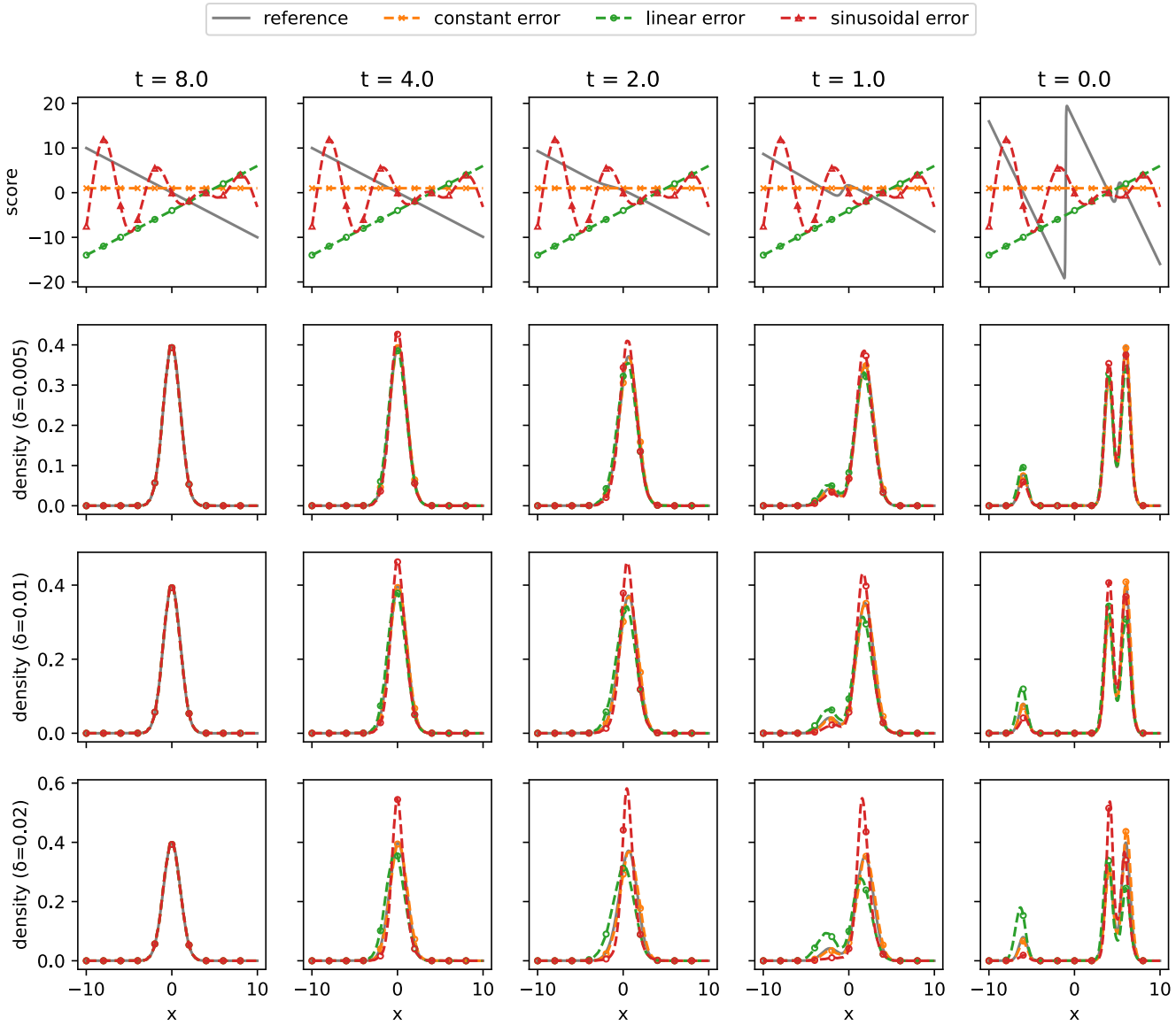
- 设置

  二阶 Heun 方法

  时间 $T = 8$, 并从 $\mathcal{N}(0, I_d)$ 初始化 4×10^4粒子

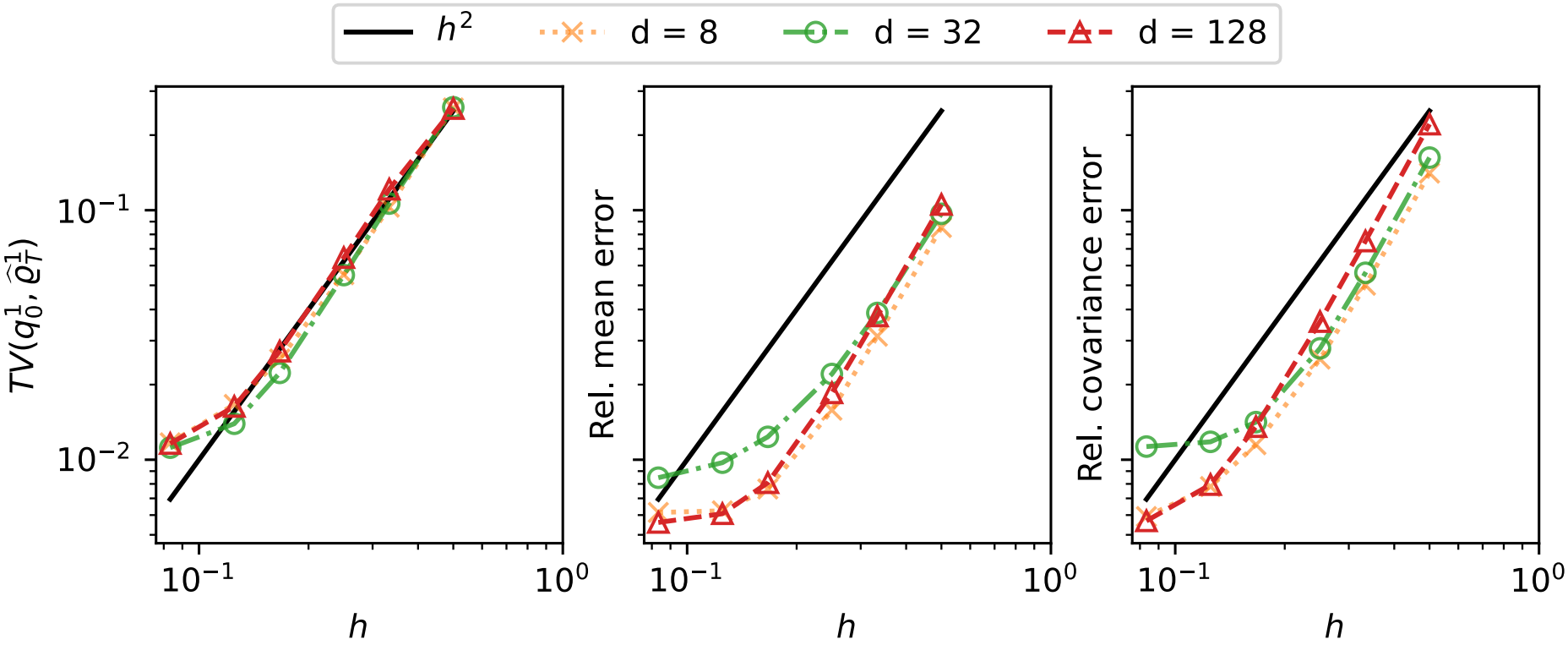
数值实验

➢ 概率密度函数演化



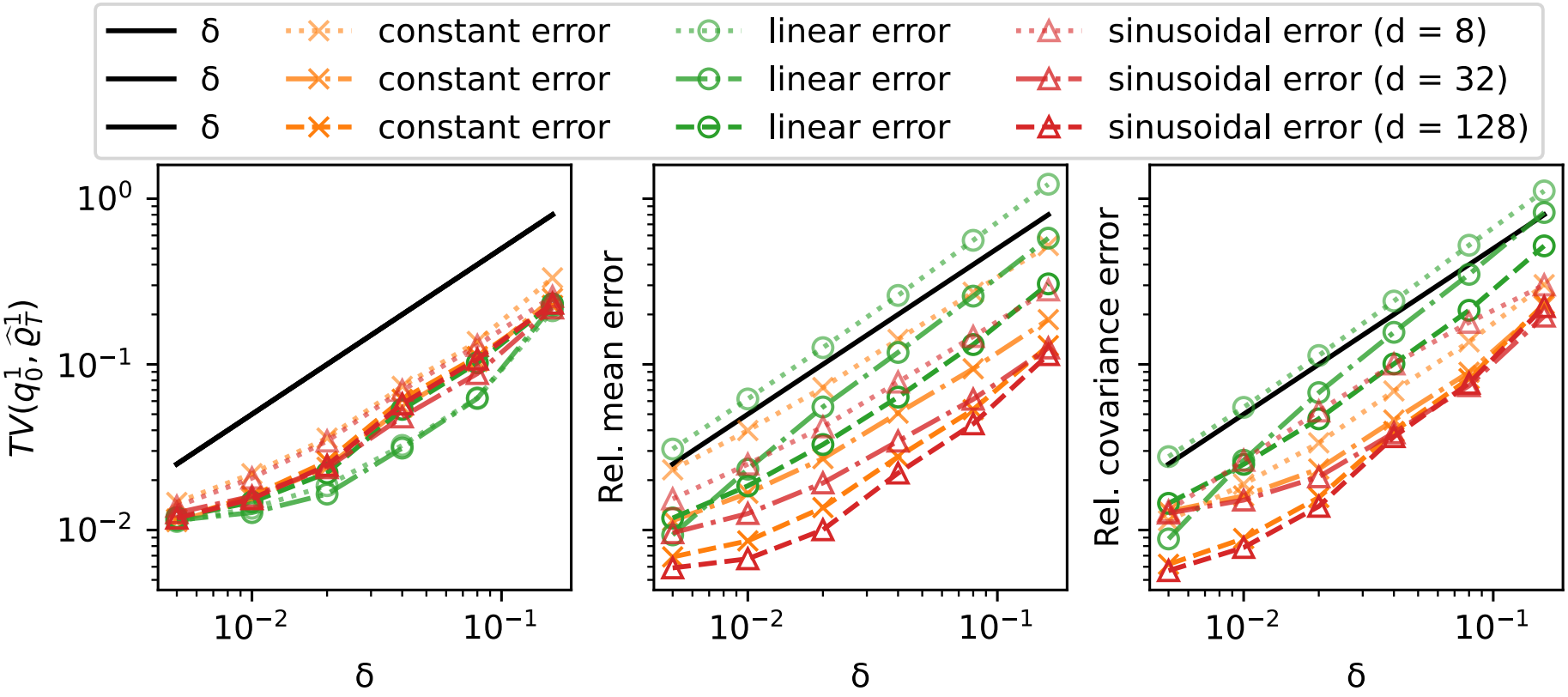
数值实验

- 离散误差 (δ=0)



数值实验

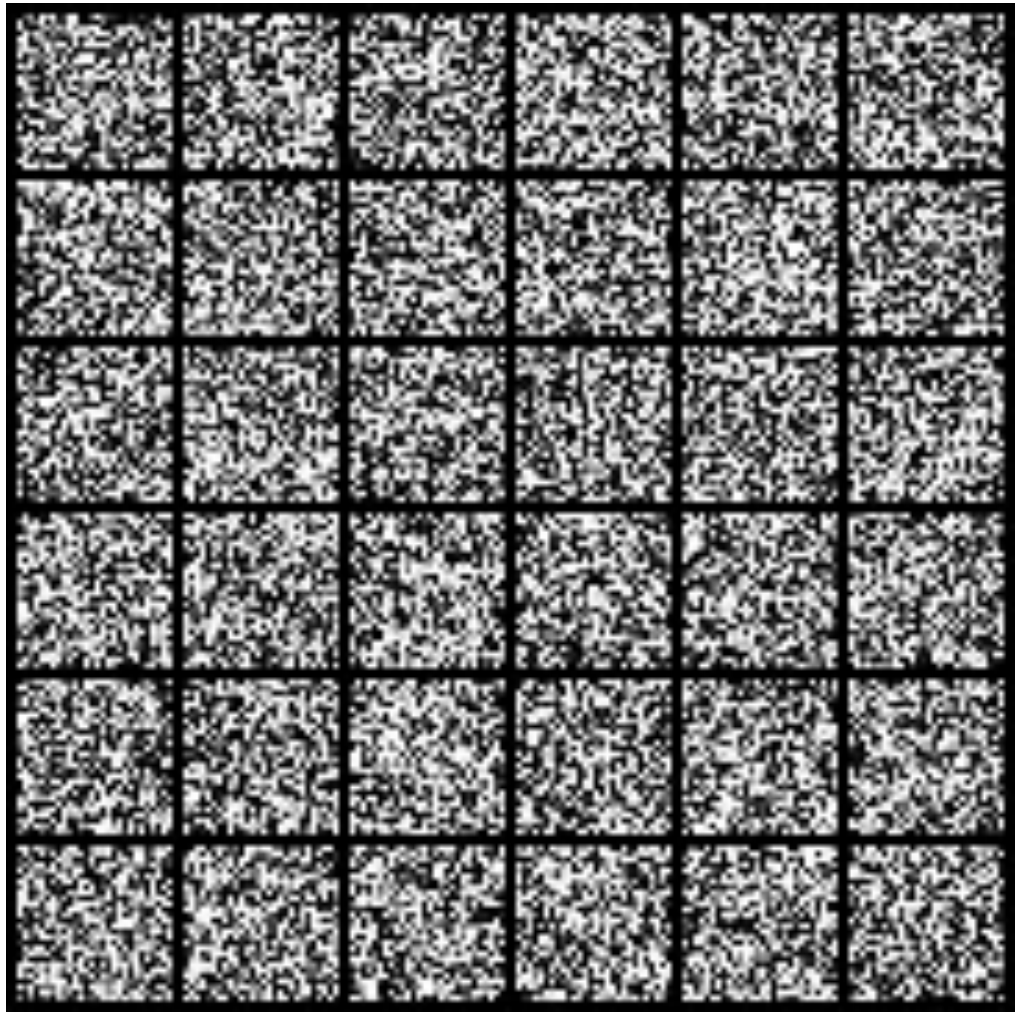
- 全变差($h^2 \approx \delta$)



- 理论误差界 $\mathcal{O}(d\sqrt{\delta} + d(dh)^p)$.
- 数值实验误差界 $\mathcal{O}(\delta + h^p)$.

数值实验

- MNIST (https://github.com/bot66/MNISTDiffusion)



扩展阅读

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