

Arbitrarily-Conditioned Multi-Functional Diffusion for Multi-Physics Emulation

ICML 2025

基于任意条件的多函数扩散模型的多物理场模拟方法

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Background & Motivation

核心任务：捕获多物理场系统之间各个函数的关系，执行多种任务（正向预测、反向推断、函数模拟）

传统物理模拟方法

eg:有限元 有限差分

优点：

理论严谨，结果可靠
能严格满足物理方程约束

缺点：

计算成本极高（如计算大型矩阵）
多物理场的系统更加复杂！
仿真一次流体可能耗时数小时甚至数天！

VS

现代机器学习代理模型

eg:FNO PINN

优点：

推理速度快
相比传统方法能降低计算成本

缺点：

不同任务需要单独训练模型
不支持不确定性量化

核心贡献

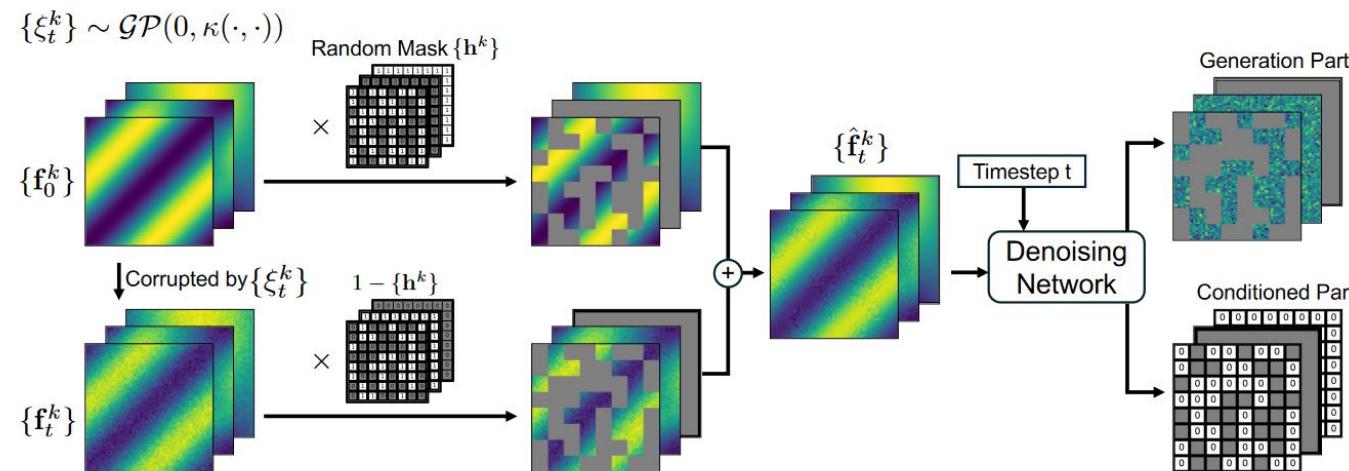
1. 多功能扩散模型

DDPM扩展到函数空间，用高斯过程建模噪声函数

$$f_t(\cdot) = \sqrt{\hat{\alpha}_t} f_0(\cdot) + \sqrt{1 - \hat{\alpha}_t} \xi_t(\cdot) \quad \xi_t \sim \mathcal{GP}(\cdot | 0, \kappa(\mathbf{z}, \mathbf{z}'))$$

2. 任意条件去噪损失

随机掩码策略，灵活处理条件生成



3. 高效训练与采样

分解核函数，使用克罗内克积，避免计算大型矩阵

(参考知乎小小将《扩散模型之DDPM》)

DDPM

随机噪声 ξ \longrightarrow 样本数据 x

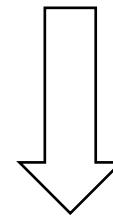


加噪 $x_0 \rightarrow x_1 \rightarrow x_2 \rightarrow x_3 \rightarrow \dots \rightarrow x_T$

去噪 $x_T \rightarrow x_{T-1} \rightarrow x_{T-2} \rightarrow x_{T-3} \rightarrow \dots \rightarrow x_0$

加噪建模 $x_t = \sqrt{\alpha_t}x_{t-1} + \sqrt{\beta_t}\varepsilon_t, \quad \varepsilon_t \sim \mathcal{N}(0, I)$

迭代 $x_{t-1} = \sqrt{\alpha_{t-1}}x_{t-2} + \sqrt{\beta_{t-1}}\varepsilon_{t-1}, \quad \varepsilon_{t-1} \sim \mathcal{N}(0, I)$



$$x_t = \sqrt{\alpha_t}x_0 + \sqrt{\beta_t}\epsilon, \quad \epsilon \sim \mathcal{N}(0, I)$$

令T步后 $\bar{\alpha}_T \approx 0$ 数据经加噪近似为高斯噪声

$$q(x_t|x_0) = \mathcal{N}(x_t; \sqrt{\alpha_t}x_0, (1 - \bar{\alpha}_t)I)$$

$$q(x_{t-1}|x_t)? \rightarrow q(x_{t-1}|x_t, x_0) = \mathcal{N}(x_{t-1}; \widehat{\mu}(x_t, x_0), \widehat{\beta}_t I)$$

$$\rightarrow q(x_{t-1}|x_t, x_0) = q(x_t|x_{t-1}, x_0) \frac{q(x_{t-1}|x_0)}{q(x_t|x_0)}$$

$$\widehat{\mu}(x_t, x_0) = \frac{\sqrt{\alpha_t}(1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t}x_t + \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1 - \bar{\alpha}_t}x_0$$

$$\widehat{\beta}_t = \frac{1 - \bar{\alpha}_{t-1}}{1 - \bar{\alpha}_t}\beta_t$$

用 x_t 估计 x_0 ?

$$\mu(x_t) = \frac{1}{\sqrt{\bar{\alpha}_t}}(x_t - \sqrt{\beta_t}\varepsilon_\theta(x_t, t))$$

$$\|x_0 - \mu(x_t)\|^2 = c\|\epsilon - \varepsilon_\theta(\sqrt{\alpha_t}x_0 + \sqrt{\beta_t}\epsilon, t)\|^2$$

随机噪声 ξ → 样本数据 x

x 是函数形式？对函数的扩散

$$x_t = \bar{\alpha}_t x_0 + \bar{\beta}_t \bar{\varepsilon}_t, \quad \bar{\varepsilon}_t \sim \mathcal{N}(0, I) \longrightarrow f_t = \bar{\alpha}_t f_0 + \bar{\beta}_t \bar{\varepsilon}_t, \quad \bar{\varepsilon}_t \sim \mathcal{GP}(0, K(z, z'))$$

原数据 $\xrightarrow{\text{加噪}}$ 高斯噪声

原函数 $\xrightarrow{\text{加噪}}$ 噪声函数

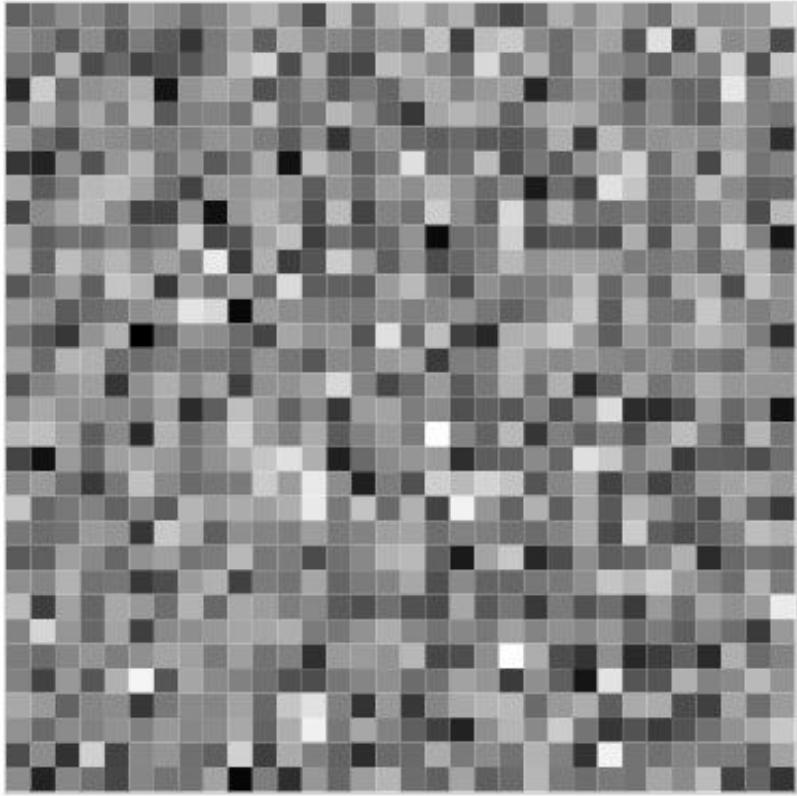
$\varepsilon_\theta(x_t, t)$

$\varepsilon_\theta(f_t, t, z)$

M个物理场
↓

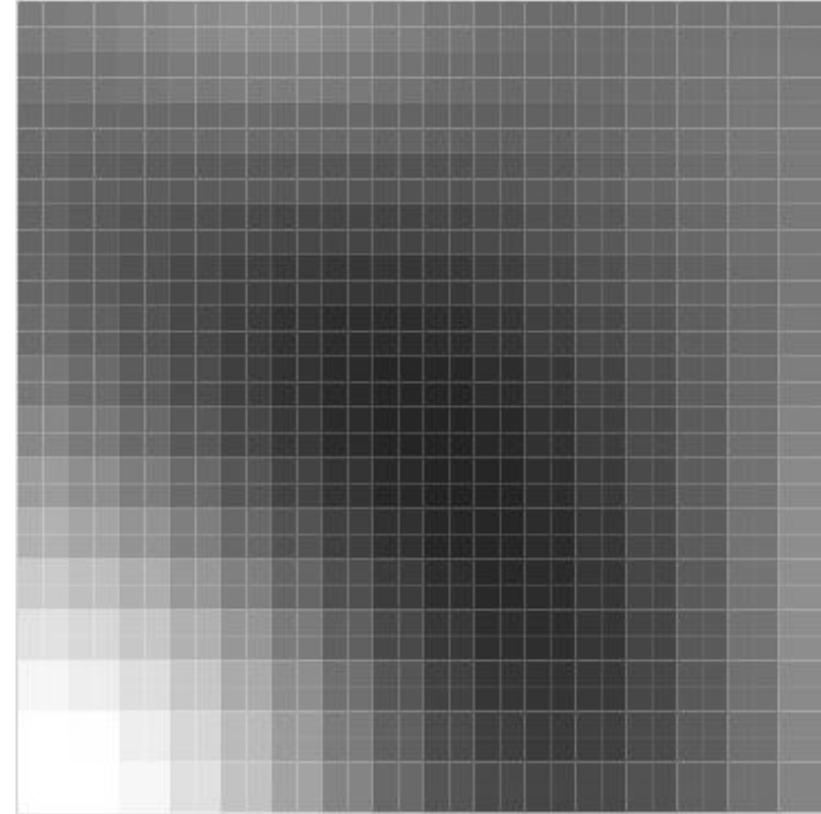
$\varepsilon_\theta(f_t^1, f_t^2, \dots, f_t^M, t, z) \xrightarrow{\text{预测}} \varepsilon_t^1, \varepsilon_t^2, \dots, \varepsilon_t^M$

普通高斯噪声



每个位置都完全独立

高斯过程噪声



$\bar{\varepsilon}_t \sim \mathcal{GP}(\mathbf{0}, \mathcal{K}(\mathbf{z}, \mathbf{z}'))$ 空间关联

M个物理场，有作为条件的，也有生成的目标

$$\varepsilon_\theta(f_t^1, f_t^2, \dots, f_t^M, t, z)$$

$$\text{条件场 } \mathcal{F}^C = \{f_0^k(\mathcal{Z}_k^C) | k \in C\}$$

$$\text{目标场 } \mathcal{F}^S = \{f_0^k(\mathcal{Z}_k^S) | k \in S\}$$

固定条件场

$$\varepsilon_\theta(\mathcal{F}^C, \mathcal{F}_t^S, t, z)$$

如何训练?

Mask机制

$$\mathcal{H} = \{h^1, h^2, \dots, h^M\} \quad \begin{matrix} h=1 \text{ 表示条件} \\ h=0 \text{ 表示目标} \end{matrix}$$

$$\nabla_\theta \|\varepsilon_\theta(\widehat{f}_t^1, \widehat{f}_t^2, \dots, \widehat{f}_t^M, t, z) - (\widehat{\varepsilon}_t^1, \widehat{\varepsilon}_t^2, \dots, \widehat{\varepsilon}_t^M)\|^2$$

$$\widehat{f}_t^k = f_0^k \circ h^k + f_t^k \circ (1 - h^k)$$

$$\widehat{\varepsilon}_t^k = 0 \circ h^k + \varepsilon_t^k \circ (1 - h^k)$$

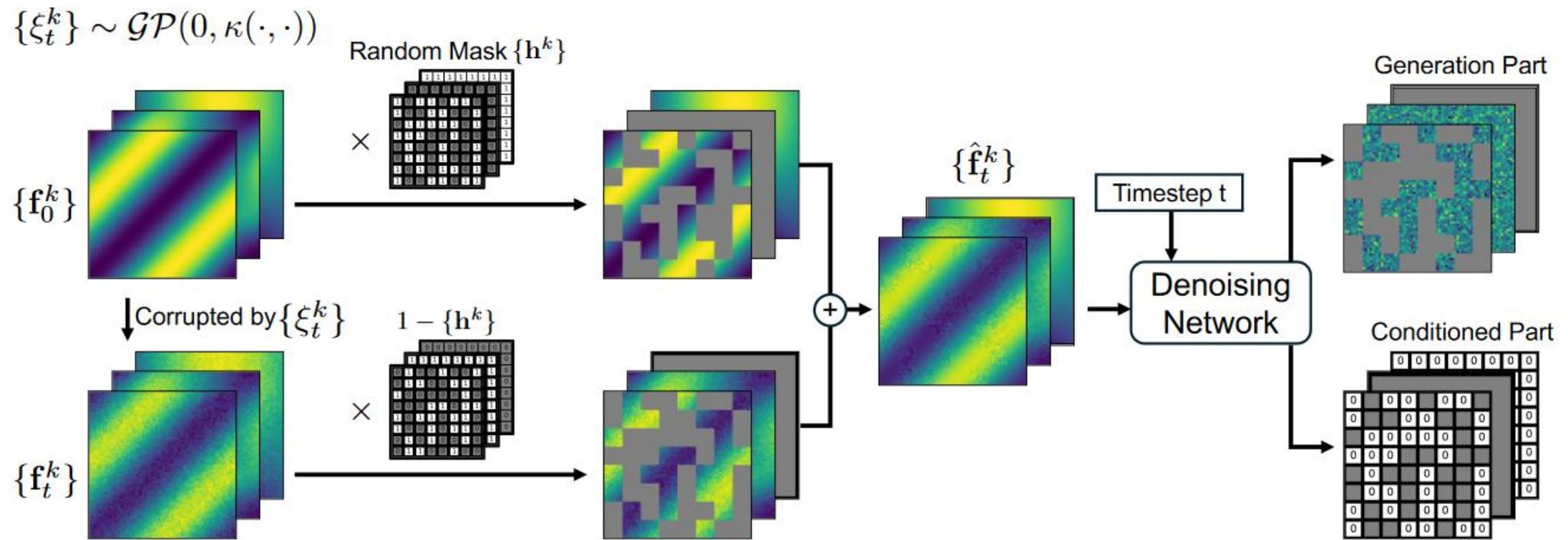
$\mathcal{F}^C = \emptyset?$ 联合生成

$\mathcal{F}^C \cap \mathcal{F}^S = \emptyset?$ 正向预测、逆问题

$\mathcal{F}^C \cap \mathcal{F}^S \neq \emptyset?$ 预测+补充观测值

训练时随机选择Mask，可以覆盖整个
函数通道，也可以对某些观测值覆盖

变换条件场和目标场的地位达到不同目的



训练流程

1、样本 $\{f_0^1, f_0^2, \dots, f_0^M\}$ 采样位置 $\{Z_k\}_{k=1}^M$

2、时间t(1 to T)

3、采样 $\{\varepsilon_t^1, \varepsilon_t^2, \dots, \varepsilon_t^M\}$ 对应 f_t^K

4、采样 $\{h_1, h_2, \dots, h_M\}$

5、 $\nabla_{\theta} ||\varepsilon_{\theta}(\widehat{f}_t^1, \widehat{f}_t^2, \dots, \widehat{f}_t^M, t, z) - (\widehat{\varepsilon}_t^1, \widehat{\varepsilon}_t^2, \dots, \widehat{\varepsilon}_t^M)||^2$

6、循环收敛

采样流程

条件场 \mathcal{F}^C
目标场 \mathcal{F}^S

1、Z上采样高斯过程 ε

2、求子集 ε 得到初始值 \mathcal{F}_T^S

3、from t=T-1, do

若 $t > 1$

Z上采样高斯过程 ε

求子集得到 $\bar{\varepsilon}$

$\varepsilon_t = \varepsilon_{\theta}(\mathcal{F}^C \cup \mathcal{F}_t^S, t, Z)$

求子集 ε_t 得到 ε_t^S

$$\mathbf{F}_{t-1}^s = \frac{1}{\sqrt{1-\beta_t}} \left(\mathbf{F}_t^s - \frac{\beta_t}{\sqrt{1-\hat{\alpha}_t}} \bar{\xi}_t^s \right) + \sqrt{\hat{\beta}_t} \bar{\epsilon}$$

4、return \mathcal{F}_0^S

$$\begin{array}{ll} \text{D-F} & -\nabla \cdot (a(\mathbf{x}) \nabla u(\mathbf{x})) = f(\mathbf{x}) \quad \mathbf{x} \in (0, 1)^2 \\ \text{Darcy-Flow} & u(\mathbf{x}) = 0, \quad \mathbf{x} \in \partial(0, 1)^2, \end{array} \quad (a, f, u)$$

$$\begin{array}{ll} \text{C-D} & \frac{\partial u(x,t)}{\partial t} + \nabla \cdot (v(x,t)u(x,t)) = D\nabla^2 u(x,t) + s(x,t), \quad (v,s,u) \\ \text{Convection Diffusion} & \end{array}$$

D-R ion Reaction	$\frac{\partial v_1}{\partial t} = D_1 \frac{\partial^2 v_1}{\partial x^2} + D_1 \frac{\partial^2 v_1}{\partial y^2} + v_1 - v_1^3 - k - v_2,$ $\frac{\partial v_2}{\partial t} = D_2 \frac{\partial^2 v_2}{\partial x^2} + D_2 \frac{\partial^2 v_2}{\partial y^2} + v_1 - v_2,$	$f_1 = v_1(2.5, x, y)$ $f_2 = v_2(2.5, x, y)$ $u_1 = v_1(5.0, x, y)$ $u_2 = v_2(5.0, x, y)$ (f_1, f_2, u_1, u_2)
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$$\begin{aligned} \text{T-F} \quad & \frac{\partial w(\mathbf{x}, t)}{\partial t} + \mathbf{u} \cdot \nabla w(\mathbf{x}, t) = \nu \nabla^2 w(\mathbf{x}, t) + f(\mathbf{x}), \quad \omega(x, t) \quad t = 2, 4, 6, 8, 10 \\ \text{Torus Fluid} \quad & w(\mathbf{x}, 0) = w_0(\mathbf{x}), \quad (\omega_0, \omega_t, f) \end{aligned}$$

实验结果（预测任务）

Dataset	Task(s)	ACM-FD	FNO	GNOT	DON	Simformer
D-F	f, u to a	1.32e-02 (2.18e-04)	1.88e-02 (1.66e-04)	1.35e-01 (6.57e-05)	2.38e-02 (3.45e-04)	1.18e-01 (3.00e-03)
	a, u to f	1.59e-02 (1.59e-04)	2.37e-02 (1.87e-04)	1.00e+00 (0.00e+00)	3.76e-02 (7.75e-04)	4.11e-02 (2.87e-03)
	a, f to u	1.75e-02 (4.16e-04)	6.29e-02 (4.18e-04)	6.09e-01 (2.40e-01)	6.05e-02 (7.17e-04)	4.04e-02 (5.17e-03)
	u to a	3.91e-02 (7.08e-04)	5.57e-02 (4.16e-04)	1.35e-01 (1.99e-04)	5.08e-02 (5.91e-04)	1.44e-01 (4.23e-03)
	u to f	3.98e-02 (6.45e-04)	5.50e-02 (5.47e-04)	9.99e-01 (7.48e-04)	6.46e-02 (1.13e-04)	1.06e-01 (3.98e-03)
C-D	s, u to v	2.17e-02 (4.53e-04)	4.50e-02 (3.89e-04)	3.26e-02 (3.41e-03)	3.64e-02 (5.07e-04)	3.96e-01 (4.79e-02)
	v, u to s	5.45e-02 (1.40e-03)	7.93e-02 (8.48e-04)	1.22e-01 (1.91e-03)	7.04e-02 (7.53e-04)	5.76e-02 (7.10e-02)
	v, s to u	1.60e-02 (2.15e-04)	7.26e-02 (2.16e-04)	5.80e-03 (1.51e-04)	7.86e-02 (7.42e-04)	1.03e-01 (1.95e-02)
	u to v	2.66e-02 (3.08e-04)	5.90e-02 (8.22e-04)	6.69e-02 (3.66e-03)	4.55e-02 (6.09e-04)	5.108e-01 (7.56e-02)
	u to s	6.06e-02 (2.54e-04)	1.16e-01 (5.63e-04)	1.85e-01 (2.84e-03)	9.65e-02 (5.52e-04)	9.21e-01 (1.00e-01)
D-R	f_1, u_1 to f_2	1.44e-02 (8.96e-04)	1.07e-02 (1.92e-04)	4.53e-01 (4.34e-02)	2.93e-01 (1.29e-03)	3.39e-02 (2.97e-03)
	f_1, u_1 to u_2	1.59e-02 (3.68e-04)	2.02e-02 (2.42e-04)	3.91e-01 (1.86e-02)	2.03e-01 (2.22e-03)	3.67e-02 (2.36e-03)
	f_2, u_2 to f_1	4.10e-02 (8.93e-04)	5.52e-02 (3.01e-03)	6.53e-01 (2.04e-02)	4.24e-01 (9.26e-04)	1.21e-01 (3.11e-03)
	f_2, u_2 to u_1	5.86e-02 (3.43e-04)	7.82e-02 (1.29e-04)	4.88e-01 (2.92e-02)	2.98e-01 (2.61e-03)	1.01e-01 (2.70e-03)
T-F	w_0, w_5 to w_1	2.73e-02 (4.78e-03)	1.28e-02 (2.38e-04)	2.40e-02 (8.74e-04)	6.32e-02 (2.72e-04)	6.14e-02 (2.44e-03)
	w_0, w_5 to w_2	2.43e-02 (1.60e-03)	2.08e-02 (9.80e-05)	4.00e-02 (5.92e-04)	7.69e-02 (4.41e-04)	6.99e-02 (2.18e-03)
	w_0, w_5 to w_3	2.43e-02 (3.17e-03)	2.33e-02 (1.83e-04)	4.74e-02 (1.23e-03)	7.34e-02 (2.88e-04)	8.34e-02 (2.60e-03)
	w_0, w_5 to w_4	1.68e-02 (1.81e-03)	1.41e-02 (1.17e-04)	3.95e-02 (6.73e-04)	5.57e-02 (1.73e-04)	9.75e-02 (3.93e-03)
	w_0, w_5 to f	1.63e-02 (1.49e-03)	1.79e-02 (3.04e-04)	5.91e-02 (4.01e-03)	4.77e-02 (5.56e-04)	1.14e-01 (4.00e-03)
	w_0, f to w_1	3.10e-02 (4.08e-03)	9.68e-03 (3.22e-04)	2.09e-02 (3.62e-04)	6.08e-02 (3.14e-04)	6.06e-02 (2.03e-03)
	w_0, f to w_2	3.28e-02 (4.79e-03)	1.70e-02 (3.51e-04)	4.15e-02 (8.21e-04)	7.73e-02 (6.18e-04)	6.18e-02 (1.02e-03)
	w_0, f to w_3	3.49e-02 (2.38e-03)	2.38e-02 (8.37e-05)	5.61e-02 (8.23e-04)	8.82e-02 (4.45e-04)	5.67e-02 (1.83e-03)
	w_0, f to w_4	3.34e-02 (3.87e-03)	3.10e-02 (1.26e-04)	6.97e-02 (1.62e-03)	1.02e-01 (7.28e-04)	4.10e-02 (1.98e-03)
	w_0, f to w_5	3.26e-02 (2.13e-03)	3.81e-02 (2.01e-04)	8.35e-02 (7.33e-04)	1.21e-01 (8.20e-04)	1.18e-01 (4.15e-03)

实验结果 (生成任务)

1000组函数平均误差

System	Task(s)	ACM-FD	MFD	β -VAE
D-F	Equation Error	0.0576	0.0584	0.265
	MRPD	1.15	0.980	0.932
C-D	Equation Error	0.114	0.127	0.282
	MRPD	1.00	0.971	0.879
T-F	Equation Error	0.0273	0.0234	0.737
	MRPD	0.8042	0.9537	0.524

实验结果 (补全任务)

Dataset	Task(s)	ACM-FD	MFD-Inpaint	Interp
D-F	<i>a</i>	1.21e-02	7.94e-02	1.04e-01
	<i>f</i>	1.23e-02	6.41e-02	6.98e-01
	<i>u</i>	1.09e-02	2.71e-02	8.07e-01
C-D	<i>v</i>	1.87e-02	4.71e-01	8.30e-01
	<i>s</i>	3.39e-02	3.22e-01	6.49e-01
	<i>u</i>	1.45e-02	3.47e-02	8.97e-01

MRPD: Mean Relative Pairwise Distance

平均相对成对距离：衡量数据生成多样性

实验结果 (不确定性量化)

重复实验100个样本

Dataset	Task	Method	0.9	0.95	0.99
C-D	s, u to v	ACM-FD	0.833	0.880	0.921
		Simformer	0.736	0.814	0.871
	v, u to s	ACM-FD	0.766	0.842	0.913
		Simformer	0.683	0.767	0.879
	v, s to u	ACM-FD	0.939	0.968	0.990
		Simformer	0.695	0.771	0.858
	u to v	ACM-FD	0.821	0.870	0.922
		Simformer	0.775	0.850	0.912
	u to s	ACM-FD	0.920	0.949	0.972
		Simformer	0.716	0.773	0.823
D-F	a, u to f	ACM-FD	0.947	0.974	0.991
		Simformer	0.829	0.895	0.950
	a, f to u	ACM-FD	0.985	0.994	0.998
		Simformer	0.922	0.955	0.998
	u to f	ACM-FD	0.867	0.909	0.952
		Simformer	0.918	0.953	0.980

$$ECP = \frac{1}{N_{\text{total}}} \sum_{i=1}^{N_{\text{total}}} \mathbb{I}(y_i \in C_\alpha)$$

附：加速采样高斯过程

1、一元高斯分布采样

$$x \sim \mathcal{N}(0, 1)$$

2、多元高斯分布采样

$$x \sim \mathcal{N}(0, \Sigma)$$

多变量不独立则不能直接分别采样独立高斯

相关性需要满足协方差矩阵 Σ



先采样 $z \sim \mathcal{N}(0, I)$

对 Σ 做 Cholesky 分解

$$\Sigma = LL^T$$

$$x = Lz$$

$$Cov(x) = E(xx^T) = LE(zz^T)L^T = LIL^T = \Sigma$$

3、高斯过程

$$f \sim \mathcal{N}(0, K)$$

在 N 个离散采样点上，为 N 维多元高斯

Cholesky 分解时间复杂度 $O(N^3)!!$



尝试降维分解核函数

附：加速采样高斯过程

$$\kappa(x, x') = \sigma^2 \exp\left(-\frac{\|x - x'\|^2}{2\ell^2}\right)$$

$$\kappa(x, x') = \sigma^2 \exp\left(-\frac{(x_1 - x'_1)^2 + (x_2 - x'_2)^2}{2\ell^2}\right)$$

$$\kappa(x, x') = \sigma^2 \exp\left(-\frac{(x_1 - x'_1)^2}{2\ell^2}\right) \exp\left(-\frac{(x_2 - x'_2)^2}{2\ell^2}\right)$$

$$\kappa(x, x') = \kappa_1(x_1, x'_1) \kappa_2(x_2, x'_2)$$

$\rightarrow K = K_1 \otimes K_2$ 克罗内克积

$$\Sigma = LL^T = (L_1 \otimes L_2)(L_1 \otimes L_2)^T$$

$$K = K_1 \otimes K_2 \otimes K_3 \otimes \dots \otimes K_D$$

$$K^{-1} = (L_1^{-1})^T L_1^{-1} \otimes \dots \otimes (L_D^{-1})^T L_D^{-1} = A^T A$$

$$A = L_1^{-1} \otimes \dots \otimes L_D^{-1}$$

$$vec(\varepsilon_t) = A^T \eta, \quad \eta \sim \mathcal{N}(0, I)$$

实际操作

1、重塑 η to $\Pi = tensor(m_1 \times \dots \times m_D)$

2、 $\varepsilon_t = \Pi \times_1 L_1^{-1} \times_2 \dots \times_D L_D^{-1}$ 模式乘

恳请批评指正

附：高斯过程

无限元高斯分布（高斯过程）

$$f(\mathbf{x}) \sim \mathcal{N}(\boldsymbol{\mu}(\mathbf{x}), \kappa(\mathbf{x}, \mathbf{x}))$$

一元高斯分布

$$p(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x - \mu)^2}{2\sigma^2}\right)$$

$$\begin{bmatrix} f(\mathbf{x}) \\ \mathbf{y}^* \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu}_f \\ \boldsymbol{\mu}_y \end{bmatrix}, \begin{bmatrix} K_{ff} & K_{fy} \\ K_{fy}^T & K_{yy} \end{bmatrix}\right)$$

其中 $K_{ff} = \kappa(\mathbf{x}, \mathbf{x})$, $K_{fy} = \kappa(\mathbf{x}, \mathbf{x}^*)$, $K_{yy} = \kappa(\mathbf{x}^*, \mathbf{x}^*)$, 则有

$$f \sim \mathcal{N}(K_{fy}^T K_{ff}^{-1} \mathbf{y} + \boldsymbol{\mu}_f, K_{yy} - K_{fy}^T K_{ff}^{-1} K_{fy})$$

多元高斯分布

$$p(\mathbf{x}) = (2\pi)^{-\frac{n}{2}} |K|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T K^{-1} (\mathbf{x} - \boldsymbol{\mu})\right)$$

$$\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, K)$$