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

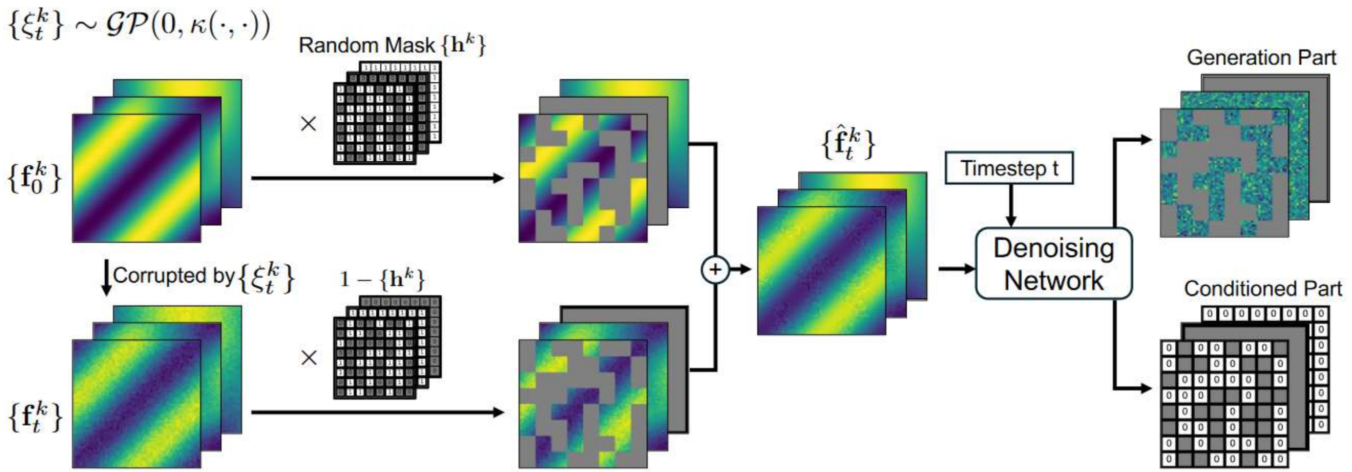
缺点：
不同任务需要单独训练模型
不支持不确定性量化

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

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

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 ⟶ 样本数据x

加噪 $x_0 \to x_1 \to x_2 \to x_3 \to \ldots \to x_T$

去噪 $x_T \to x_{T-1} \to x_{T-2} \to x_{T-3} \to \ldots \to x_0$

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

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

⇓

$$x_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}(x_t - \sqrt{\bar{\beta}_t}\epsilon)$$

$$x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{\bar{\beta}_t}\epsilon, \epsilon \sim \mathcal{N}(0, I)$$

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

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

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

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

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

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

用x_t估计x_0？

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

$$\|x_0 - \mu(x_t)\|^2 = c\left\|\epsilon - \varepsilon_\theta(\sqrt{\bar{\alpha}_t}x_0 + \sqrt{\bar{\beta}_t}\epsilon, t)\right\|^2$$

随机噪声$\xi \longrightarrow$ 样本数据x

x是函数形式？对函数的扩散

$$x_t = \overline{\alpha_t} x_0 + \overline{\beta_t}\,\bar{\varepsilon}_t, \qquad \bar{\varepsilon}_t \sim \mathcal{N}(0, I) \longrightarrow f_t = \overline{\alpha_t} f_0 + \overline{\beta_t}\,\bar{\varepsilon}_t, \qquad \bar{\varepsilon}_t \sim \overset{\text{高斯过程}}{\mathcal{GP}}(0, \mathcal{K}(z, z'))$$

原数据 $\xrightarrow{\text{加噪}}$ 高斯噪声

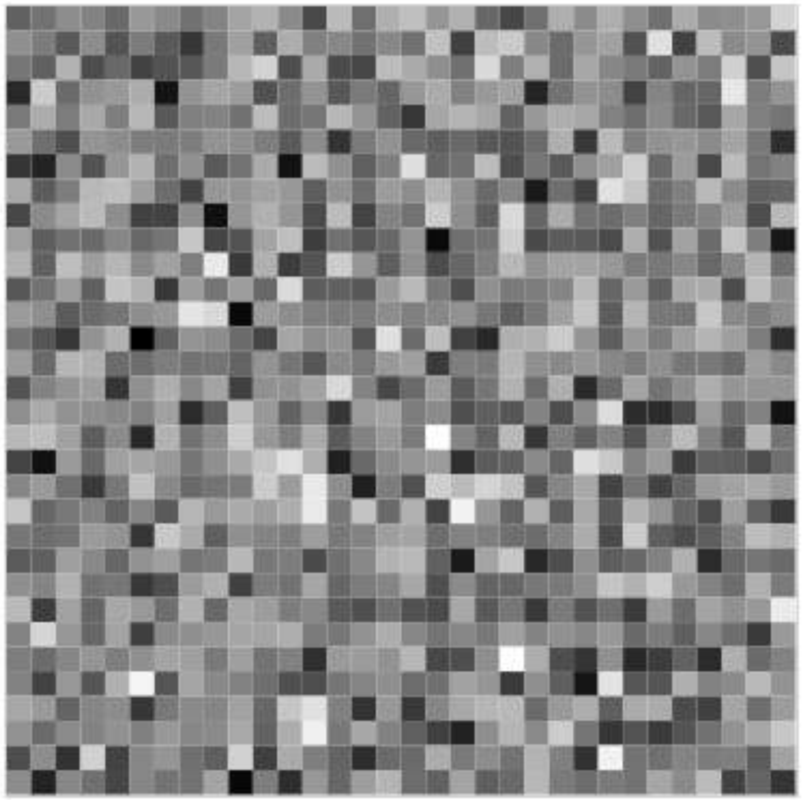
原函数 $\xrightarrow{\text{加噪}}$ 噪声函数

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

$$\Big\downarrow \text{M个物理场}$$

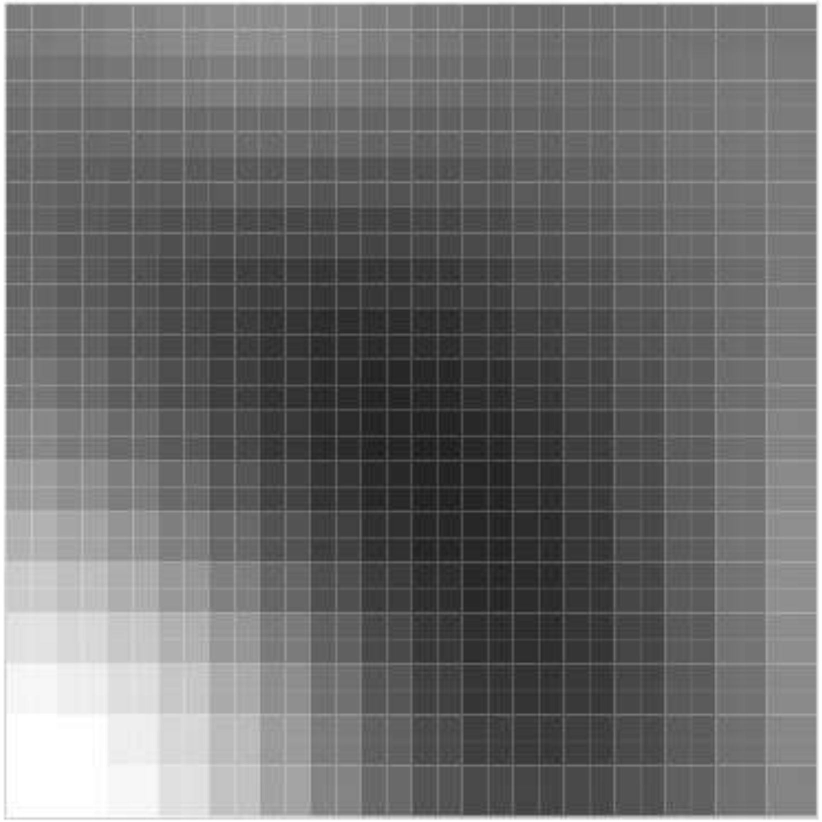
$$\varepsilon_\theta(f_t^1, f_t^2, \dots, f_t^M, t, z) \xrightarrow{\text{预测}} \varepsilon_t^1, \varepsilon_t^2, \dots, \varepsilon_t^M$$

普通高斯噪声



每个位置都完全独立

高斯过程噪声



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

M个物理场，有作为条件的，也有生成的目标

$\boldsymbol{\varepsilon}_\theta(f_t^1, f_t^2, \ldots, f_t^M, t, z)$

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

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

固定条件场

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

如何训练?

Mask机制

$\mathcal{H} = \{h^1, h^2, \ldots, h^M\}$

h=1表示条件

h=0表示目标

$$\nabla_\theta \| \boldsymbol{\varepsilon}_\theta\left(\widehat{f_t^1}, \widehat{f_t^2}, \ldots, \widehat{f_t^M}, t, z\right) - (\widehat{\varepsilon_t^1}, \widehat{\varepsilon_t^2}, \ldots, \widehat{\varepsilon_t^M}) \|^2$$

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

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

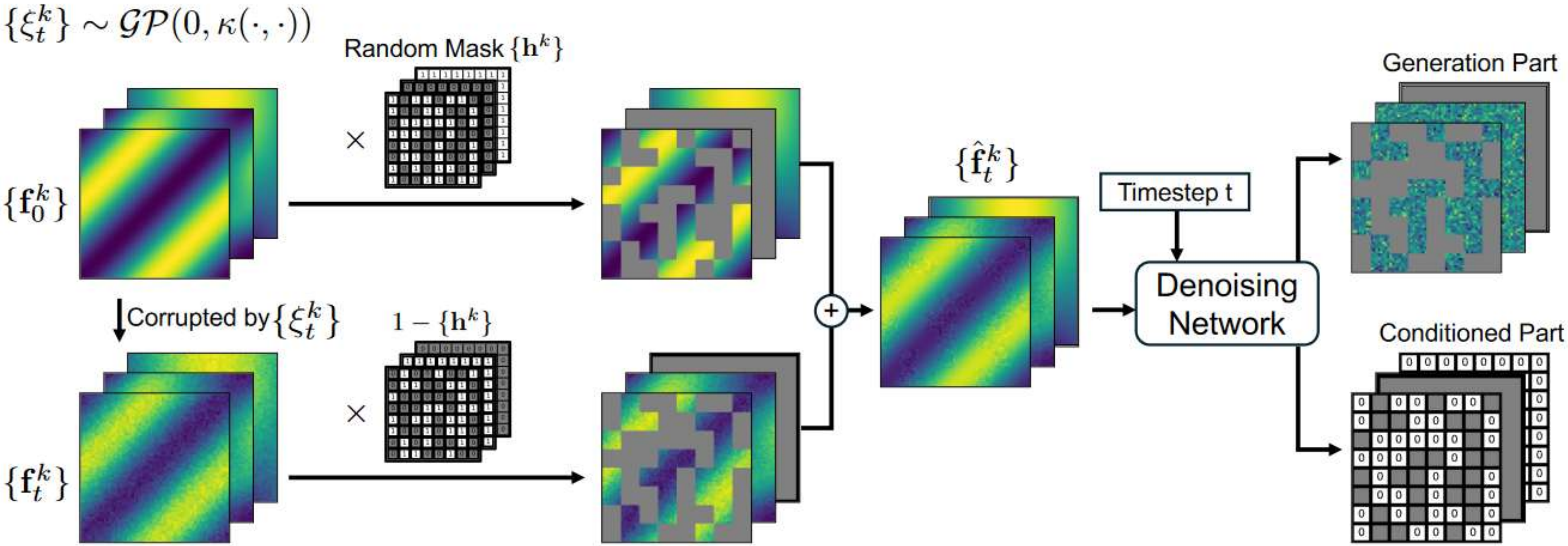
训练时随机选择Mask，可以覆盖整个函数通道，也可以对某些观测值覆盖

$\mathcal{F}^C = \emptyset$? 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

变换条件场和目标场的地位达到不同目的


$\{\xi_t^k\} \sim \mathcal{GP}(0, \kappa(\cdot,\cdot))$
Random Mask $\{\mathbf{h}^k\}$
$\times$
$\{\mathbf{f}_0^k\}$
Corrupted by $\{\xi_t^k\}$
$1 - \{\mathbf{h}^k\}$
$\times$
$\{\mathbf{f}_t^k\}$
$\{\hat{\mathbf{f}}_t^k\}$
Timestep t
Denoising Network
Generation Part
Conditioned Part

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、$\nabla_\theta ||\varepsilon_\theta\left(\widehat{f_t^1}, \widehat{f_t^2}, \dots, \widehat{f_t^M}, t, z\right) - (\widehat{\varepsilon_t^1}, \widehat{\varepsilon_t^2}, \dots, \widehat{\varepsilon_t^M})||^2$

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

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

4、return $\mathcal{F}_0^S$

D-F
Darcy-Flow

$$-\nabla \cdot (a(\mathbf{x})\nabla u(\mathbf{x})) = f(\mathbf{x}) \quad \mathbf{x} \in (0,1)^2$$
$$u(\mathbf{x}) = 0, \quad \mathbf{x} \in \partial(0,1)^2,$$

(a, f, u)

C-D
Convection Diffusion

$$\frac{\partial u(x,t)}{\partial t} + \nabla \cdot (v(x,t)u(x,t)) = D\nabla^2 u(x,t) + s(x,t),$$

(v, s, u)

D-R

Diffusion 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)

T-F

Torus Fluid

$$\frac{\partial w(\mathbf{x},t)}{\partial t} + \mathbf{u} \cdot \nabla w(\mathbf{x},t) = \nu \nabla^2 w(\mathbf{x},t) + f(\mathbf{x}),$$
$$w(\mathbf{x},0) = w_0(\mathbf{x}),$$

$\omega(x,t)\ \ t = 2,4,6,8,10$

(ω_0, ω_t, f)

1000train 100val 200test

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)	5.108-01 (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

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（补全任务）

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

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

$\downarrow$

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$\boldsymbol{O}(\boldsymbol{N}^3)$!!

$\downarrow$

尝试降维分解核函数

附：加速采样高斯过程

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

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

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

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

$K = K_1 \otimes K_2$ **克罗内克积**

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

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

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

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

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

实际操作

1、重塑$\eta\ \ to\ \ \Pi = tensor(m_1 \times \cdots \times m_D)$

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

恳请批评指正

附：高斯过程

一元高斯分布

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

多元高斯分布

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

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

无限元高斯分布（高斯过程）

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

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

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

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