

无监督聚类启发的非刚性点集配准

赵明阳
中国科学院香港创新研究院
2024年8月1日

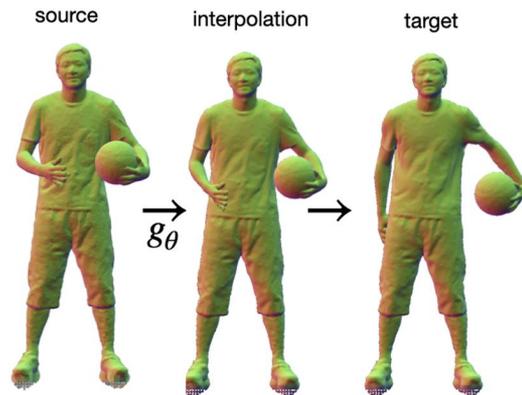
非刚性配准的应用——几何



动态重建[1]



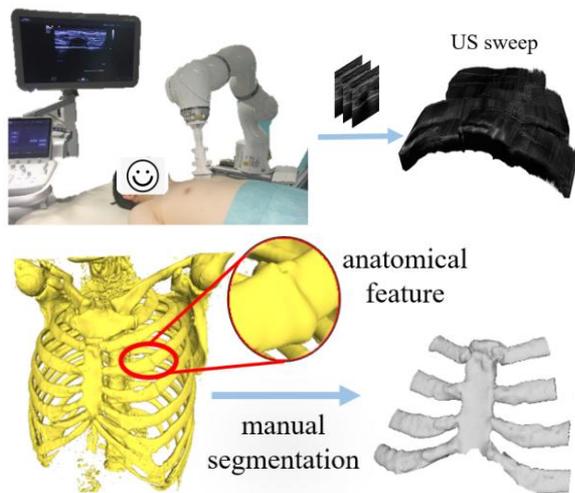
形状补全[2]



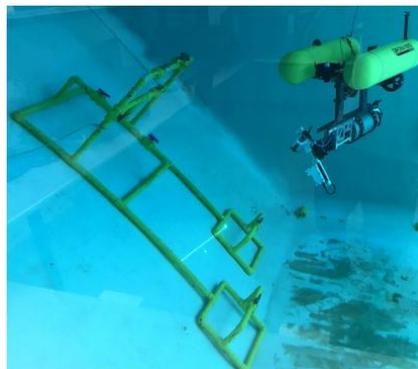
形状插值[3]

- [1] Yao et al. DynoSurf: Neural Deformation-based Temporally Consistent Dynamic Surface Reconstruction, ECCV, 2024
- [2] Halimi et al. Towards Precise Completion of Deformable Shapes, ECCV, 2020
- [3] Prokudin et al. Towards Efficient and Scalable Dynamic Surface Representations, ICCV, 2023

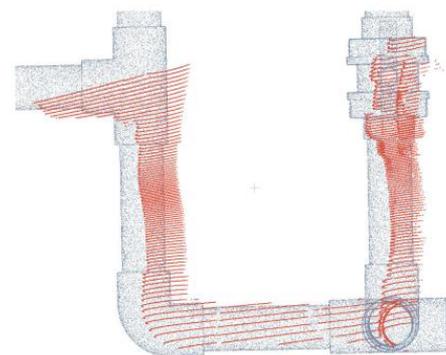
非刚性配准的应用——机器人



超声机器人 [1]

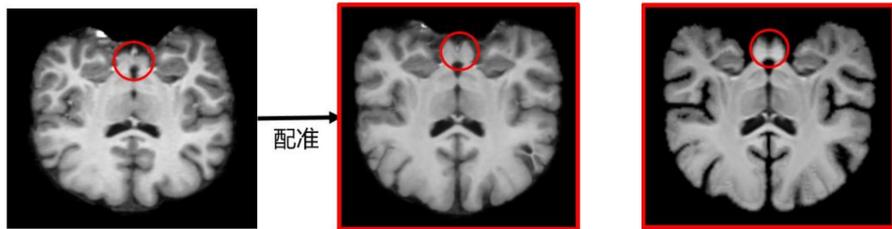
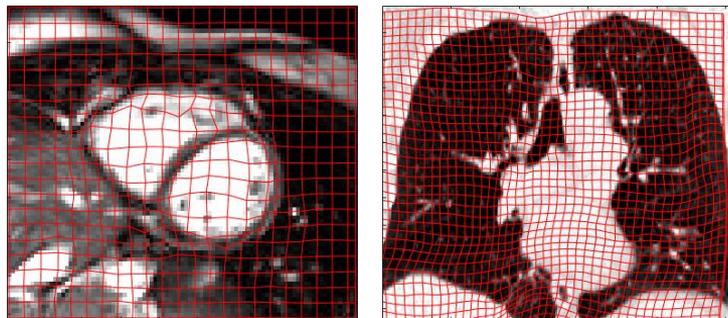


水下机器人 [2]



- [1] Jiang et al. Skeleton Graph-based Ultrasound-CT Non-rigid Registration, RAL, 2023
[2] Castellón et al. Linewise Non-Rigid Point Cloud Registration, RAL, 2022

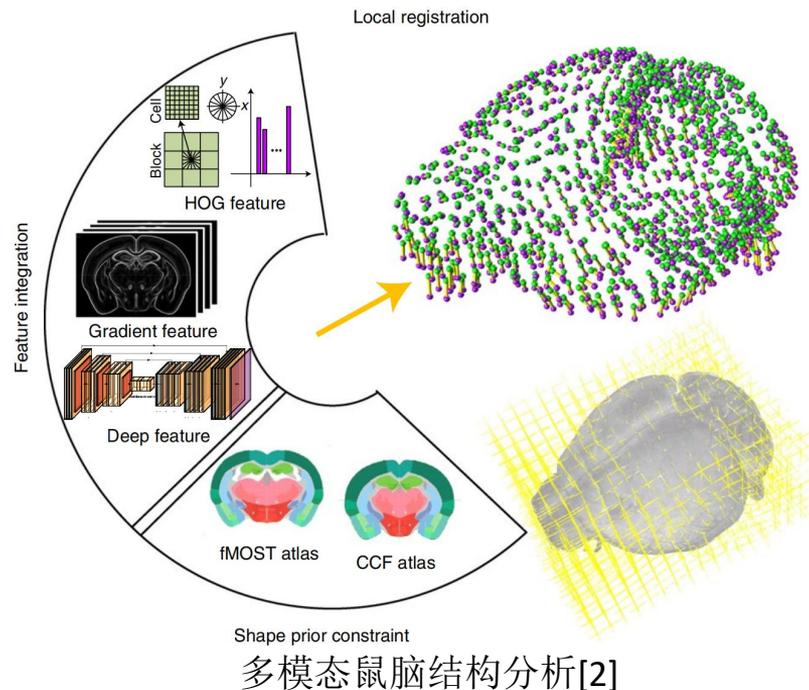
非刚性配准的应用——生物医学成像



某病人被治疗后

健康人模板

医学诊断[1]



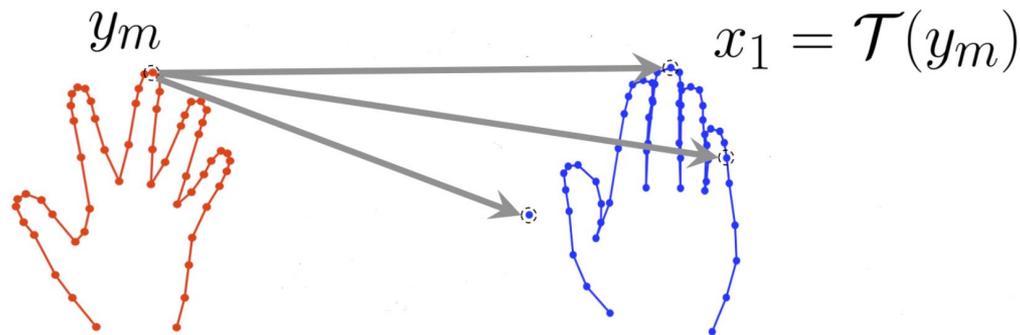
[1] <https://bbs.huaweicloud.com/blogs/174612>

[2] Qu et al. Cross-modal coherent registration of whole mouse brains, Nature Methods, 2021

非刚性配准的定义

Target: $\mathbf{X} = \{x_i \in \mathbb{R}^n\}_{i=1}^N$

Source: $\mathbf{Y} = \{y_m \in \mathbb{R}^n\}_{m=1}^M$



优化目标:

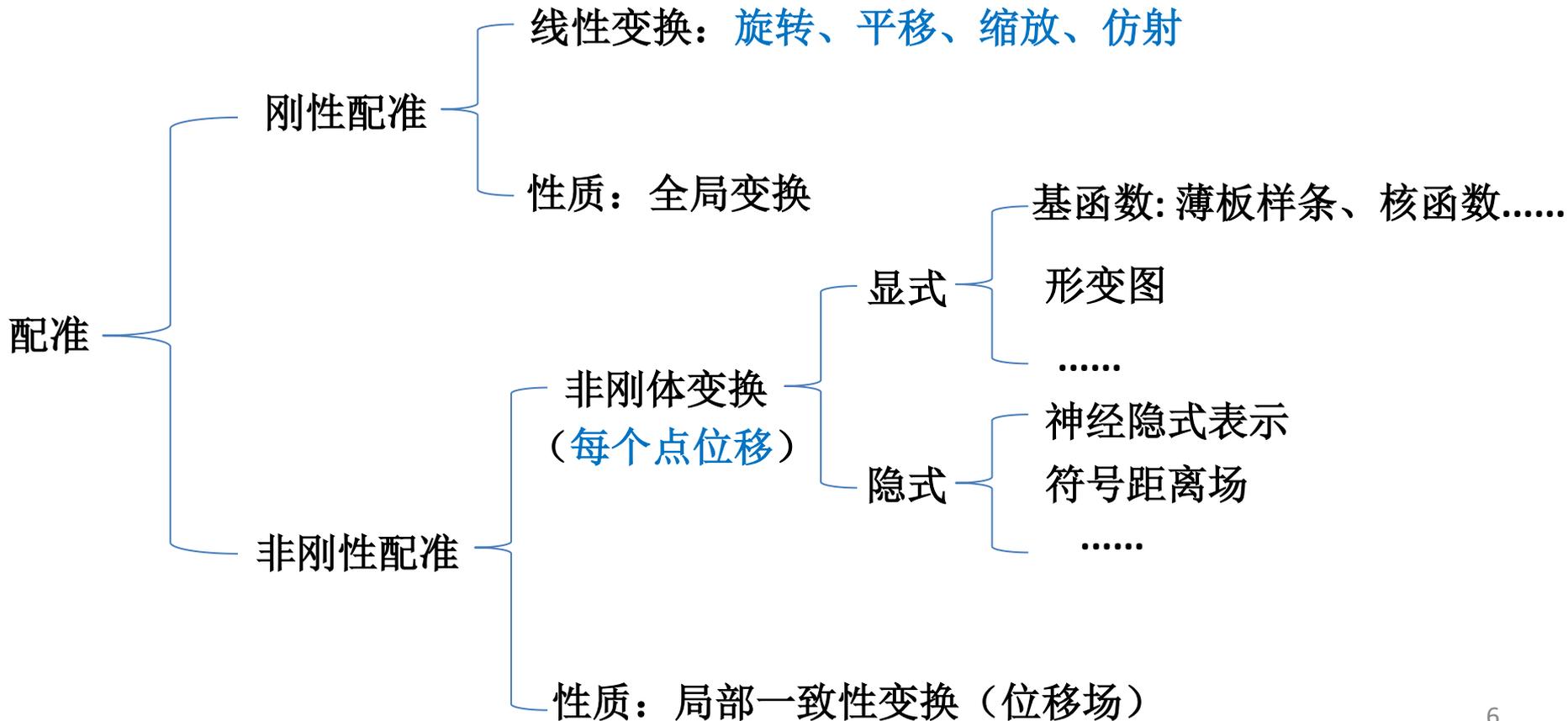
映射
或形变场

\mathcal{T}
 ν

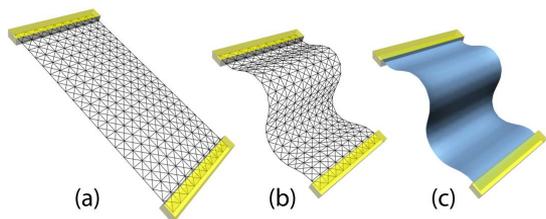
$$x_i = \mathcal{T}(y_m) = y_m + \nu(y_m)$$

为每个点求其形变(位移)量

非刚性配准的刻画

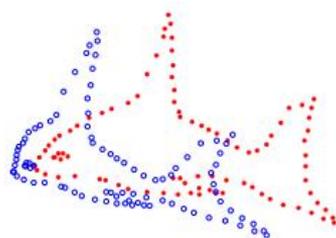


非刚性配准的刻画



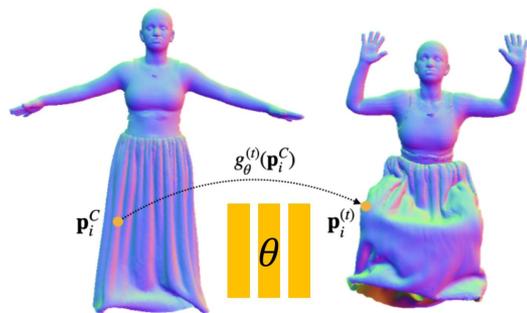
$$\hat{y}_m = \sum_{p_j \in \mathcal{I}(y_m)} \omega_{ij} \cdot (\mathbf{A}_j (y_m - p_j) + p_j + \mathbf{t}_j)$$

形变图[1]



$$\nu(y) = \sum_{m=1}^M w_m \mathcal{G}(y - y_m)$$

核函数[2]



$$\hat{y}_m = y_m + g_\theta(y_m)$$

神经隐式表示[3]

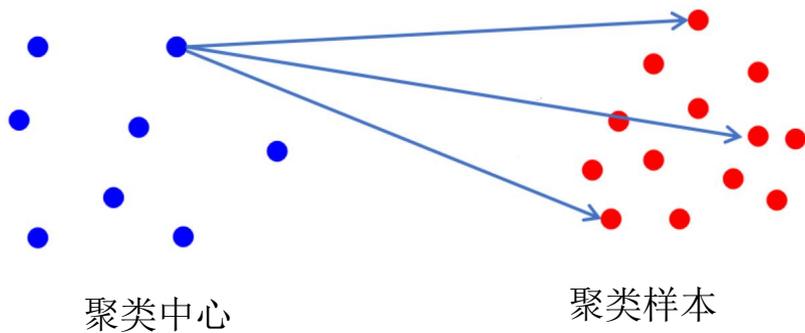
[1] Sumner et al. Embedded Deformation for Shape Manipulation, Siggraph, 2007

[2] Hirose et al. A Bayesian Formulation of Coherent Point Drift, TPAMI, 2020

[3] Prokudin et al. Towards Efficient and Scalable Dynamic Surface Representations, ICCV, 2023

无监督聚类启发的非刚性配准

1. 将非刚性配准问题转化为无监督聚类过程
2. 尝试解决大形变问题



聚类过程：聚类中心位置更新



大形变

无监督聚类启发的非刚性配准

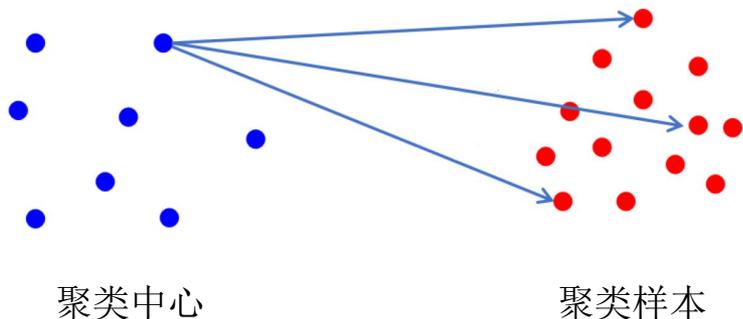
$$\min_{\mathbf{U}, \mathbf{V}} J(\mathbf{U}, \mathbf{V}) = \sum_{j=1}^C \sum_{i=1}^M (u_{ij})^r \|\mathbf{x}_i - \mathbf{v}_j\|_2^2,$$

$$s.t. \quad \sum_{j=1}^C u_{ij} = 1, \quad u_{ij} \in (0, 1]$$



$$\min_{\mathbf{U}, \mathbf{V}, \alpha} J(\mathbf{U}, \mathbf{V}, \alpha) = \sum_{j=1}^C \sum_{i=1}^M (u_{ij})^r \|\mathbf{x}_i - \mathbf{v}_j\|_2^2 + \lambda u_{ij} \log\left(\frac{u_{ij}}{\alpha_j}\right),$$

$$s.t. \quad \sum_{j=1}^C u_{ij} = 1, \quad \sum_{j=1}^C \alpha_j = 1, \quad u_{ij}, \alpha_j \in (0, 1]$$



模糊聚类

$$\min_{\mathbf{U}, \mathbf{V}, \Sigma, \alpha} J(\mathbf{U}, \mathbf{V}, \Sigma, \alpha) = \sum_{j=1}^C \sum_{i=1}^M (u_{ij})^r \|\Sigma_j^{-\frac{1}{2}} (\mathbf{x}_i - \mathbf{v}_j)\|_2^p$$

$$+ u_{ij} \log |\Sigma_j| + \lambda u_{ij} \log \frac{u_{ij}}{\alpha_j},$$

$$s.t. \quad \sum_{j=1}^C u_{ij} = 1, \quad \sum_{j=1}^C \alpha_j = 1, \quad u_{ij}, \alpha_j \in (0, 1].$$

$$\mathbf{U} = [u_{ij}]_{M \times C} \in \mathbb{R}^{M \times C}$$

$$\Sigma_j \in \mathbb{S}_{++}^n \triangleq \{\mathbf{A} \in \mathbb{R}^{n \times n} \mid \mathbf{x}^T \mathbf{A} \mathbf{x} > 0, \forall \mathbf{x} \in \mathbb{R}^n\}$$

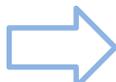
无监督聚类启发的非刚性配准

非刚性配准

$$\begin{aligned} \min_{\mathbf{U}, \alpha, \Sigma, \nu} J(\mathbf{U}, \alpha, \Sigma, \nu) &= \sum_{j=1}^C \sum_{i=1}^M u_{ij} \|\Sigma_j^{-\frac{1}{2}} (\mathbf{x}_i - (\mathbf{y}_j + \nu(\mathbf{y}_j)))\|_2^2 \\ &\quad + u_{ij} \log |\Sigma_j| + \lambda u_{ij} \log \frac{u_{ij}}{\alpha_j}, \\ \text{s.t. } |\Sigma_j| &= \theta_j, \sum_{j=1}^C u_{ij} = 1, \sum_{j=1}^C \alpha_j = 1, u_{ij}, \alpha_j \in (0, 1]. \end{aligned}$$

Source: $\mathbf{Y} = \{\mathbf{y}_j \in \mathbb{R}^n\}_{j=1}^N$  聚类中心

Target: $\mathbf{X} = \{\mathbf{x}_i \in \mathbb{R}^n\}_{i=1}^M$  聚类样本

形变: $\mathcal{T}(\mathbf{Y}) \triangleq \mathbf{Y} + \nu(\mathbf{Y})$  更新聚类中心

Source 形变到 Target 的配准问题等价于聚类中心更新过程

无监督聚类启发的非刚性配准

理论分析

1. 信息论角度：熵正则避免 \mathbf{U} 过度稀疏

$$\min_{\mathbf{U}, \boldsymbol{\alpha}, \boldsymbol{\Sigma}, \nu} J(\mathbf{U}, \boldsymbol{\alpha}, \boldsymbol{\Sigma}, \nu) = \sum_{j=1}^C \sum_{i=1}^M u_{ij} \|\boldsymbol{\Sigma}_j^{-\frac{1}{2}} (\mathbf{x}_i - (\mathbf{y}_j + \nu(\mathbf{y}_j)))\|_2^2 + u_{ij} \log |\boldsymbol{\Sigma}_j| + \lambda u_{ij} \log \frac{u_{ij}}{\alpha_j},$$

 $H(\mathbf{U}) = -\sum_{j=1}^C \sum_{i=1}^M u_{ij} \log(u_{ij})$

$$\sum_{j=1, i=1}^{C, M} u_{ij} \|\boldsymbol{\Sigma}_j^{-\frac{1}{2}} (\mathbf{x}_i - (\mathbf{y}_j + \nu(\mathbf{y}_j)))\|_2^2 + u_{ij} \log \left(\frac{|\boldsymbol{\Sigma}_j|}{\alpha_j^\lambda} \right) - \lambda H(\mathbf{U})$$

无监督聚类启发的非刚性配准

理论分析

2. 优化角度: $u_{ij} \log(u_{ij})$ 凸化目标函数, 尽量避免局部最优解

$$\min_{\mathbf{U}, \boldsymbol{\alpha}, \boldsymbol{\Sigma}, \nu} J(\mathbf{U}, \boldsymbol{\alpha}, \boldsymbol{\Sigma}, \nu) = \sum_{j=1}^C \sum_{i=1}^M u_{ij} \|\boldsymbol{\Sigma}_j^{-\frac{1}{2}} (\mathbf{x}_i - (\mathbf{y}_j + \nu(\mathbf{y}_j)))\|_2^2 + u_{ij} \log |\boldsymbol{\Sigma}_j| + \lambda u_{ij} \log \frac{u_{ij}}{\alpha_j},$$

$$\nabla^2 f(u_{ij}) = \nabla^2 u_{ij} \log(u_{ij}) = \frac{1}{u_{ij}} > 0$$

$u_{ij} \log(u_{ij})$ 罚函数, 避免 $u_{ij} \notin (0, 1]$

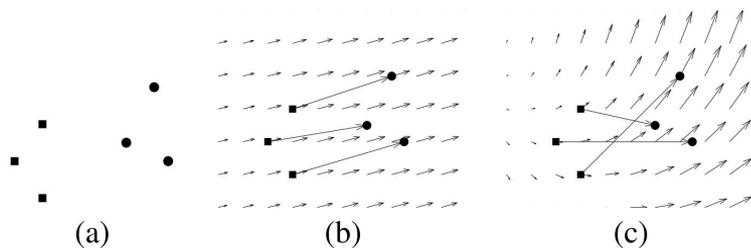
无监督聚类启发的非刚性配准

正则化

Tikhonov 正则化，使得形变场光滑

$$\min_{\mathbf{U}, \boldsymbol{\alpha}, \boldsymbol{\Sigma}, \nu} J(\mathbf{U}, \boldsymbol{\alpha}, \boldsymbol{\Sigma}, \nu) + \zeta \mathcal{R}(\nu)$$

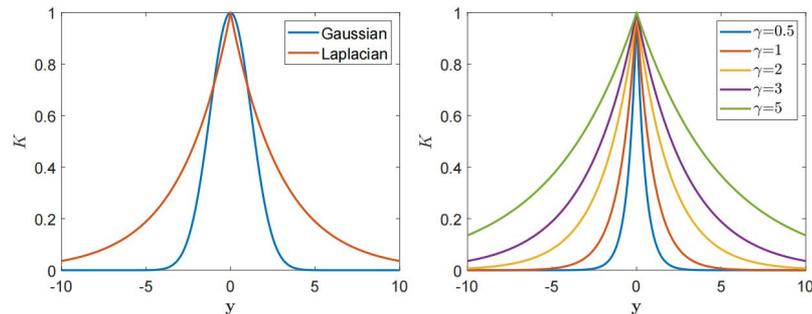
$$\mathcal{R}(\nu) = \int_{\mathbf{R}^n} ds \frac{\|\tilde{\nu}(\mathbf{s})\|_2^2}{\tilde{K}(\mathbf{s})}$$



运动一致性[1]

Laplace 核函数

$$K(\mathbf{y}_i, \mathbf{y}_j) = \exp(-\gamma \|\mathbf{y}_i - \mathbf{y}_j\|_1), \quad \gamma > 0$$



Laplace VS. Gauss

无监督聚类启发的非刚性配准

解析解

$$\min_{\mathbf{U}, \boldsymbol{\alpha}, \boldsymbol{\Sigma}, \nu} J(\mathbf{U}, \boldsymbol{\alpha}, \boldsymbol{\Sigma}, \nu) + \zeta \mathcal{R}(\nu)$$

$$s.t. |\boldsymbol{\Sigma}_j| = \theta_j, \sum_{j=1}^C u_{ij} = 1, \sum_{j=1}^C \alpha_j = 1, u_{ij}, \alpha_j \in (0, 1]$$

$$J(\mathbf{U}, \boldsymbol{\alpha}, \boldsymbol{\Sigma}, \nu) = \sum_{j=1}^C \sum_{i=1}^M u_{ij} \|\boldsymbol{\Sigma}_j^{-\frac{1}{2}} (\mathbf{x}_i - (\mathbf{y}_j + \nu(\mathbf{y}_j)))\|_2^2 \\ + u_{ij} \log |\boldsymbol{\Sigma}_j| + \lambda u_{ij} \log \frac{u_{ij}}{\alpha_j}$$



虽然目标函数非凸，但对每个未知变量可导出其解析解



直接交替优化或坐标下降法即可

无监督聚类启发的非刚性配准

解析解--更新U

$$\begin{aligned} & \min_{\mathbf{U}, \boldsymbol{\alpha}, \boldsymbol{\Sigma}, \nu} J(\mathbf{U}, \boldsymbol{\alpha}, \boldsymbol{\Sigma}, \nu) + \zeta \mathcal{R}(\nu) \\ & \text{s.t. } |\boldsymbol{\Sigma}_j| = \theta_j, \sum_{j=1}^C u_{ij} = 1, \sum_{j=1}^C \alpha_j = 1, u_{ij}, \alpha_j \in (0, 1] \\ & J(\mathbf{U}, \boldsymbol{\alpha}, \boldsymbol{\Sigma}, \nu) = \sum_{j=1}^C \sum_{i=1}^M u_{ij} \|\boldsymbol{\Sigma}_j^{-\frac{1}{2}}(\mathbf{x}_i - (\mathbf{y}_j + \nu(\mathbf{y}_j)))\|_2^2 \\ & \quad + u_{ij} \log |\boldsymbol{\Sigma}_j| + \lambda u_{ij} \log \frac{u_{ij}}{\alpha_j} \end{aligned}$$

$$\begin{aligned} \mathcal{L}(\mathbf{U}, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{\eta}) = & \sum_{j=1}^C \sum_{i=1}^M u_{ij} \|\boldsymbol{\Sigma}_j^{-\frac{1}{2}}(\mathbf{x}_i - (\mathbf{y}_j + \nu(\mathbf{y}_j)))\|_2^2 \\ & + u_{ij} \log |\boldsymbol{\Sigma}_j| + \lambda u_{ij} \log \frac{u_{ij}}{\alpha_j} + \sum_{i=1}^M \beta_i (\sum_{j=1}^C u_{ij} - 1) \\ & + \sum_{j=1}^C \sum_{i=1}^M \gamma_{ij} (u_{ij} - 1) + \sum_{j=1}^C \sum_{i=1}^M \eta_{ij} (-u_{ij}), \end{aligned}$$

$$\left\{ \begin{aligned} & \sum_{i,j=1}^{M,C} (\|\boldsymbol{\Sigma}_j^{-\frac{1}{2}}(\mathbf{x}_i - (\mathbf{y}_j + \nu(\mathbf{y}_j)))\|_2^2 + \log |\boldsymbol{\Sigma}_j| \\ & + \lambda (\log \frac{u_{ij}}{\alpha_j} + 1) + \gamma_{ij} - \eta_{ij}) + C \sum_{i=1}^M \beta_i = 0, \\ & \sum_{j=1}^C u_{ij} - 1 = 0, \quad u_{ij-1} \leq 0, \quad -u_{ij} < 0, \\ & \gamma_{ij} \geq 0, \quad \eta_{ij} \geq 0, \quad \gamma_{ij}(u_{ij-1}) = 0, \quad \eta_{ij}(-u_{ij}) = 0. \end{aligned} \right.$$



$$\mathbf{U} = (\text{diag}(\mathbf{A} \mathbf{1}_C))^{-1} \mathbf{A}$$

$$\mathbf{A} = \exp(-\mathbf{D}/\lambda) \text{diag}(\boldsymbol{\alpha} \odot |\boldsymbol{\Sigma}|)$$

无监督聚类启发的非刚性配准

更新 α

$$\alpha = \frac{1}{M} \mathbf{U}^T \mathbf{1}_M$$

更新 Σ

$$\sigma^2 = \frac{\text{tr}(\mathbf{X}^T \text{diag}(\mathbf{U}^T \mathbf{1}_M) \mathbf{X} - (2(\mathbf{U}\mathbf{X})^T + \mathbf{T}^T \text{diag}(\mathbf{U}\mathbf{1}_C)) \mathbf{T})}{n \times M}$$

无监督聚类启发的非刚性配准

更新 ν

$$\nu(\mathbf{y}) = \sum_{j=1}^C c_j K(\mathbf{y}, \mathbf{y}_j) + \sum_{\eta=1}^N d_{\eta} \psi_{\eta}(\nu)$$

$\{\psi_{\eta}\}_{\eta=1}^N$ 是 RKHS Null空间中的基函数

由于Laplace Kernel 正定, $\psi_{\eta} \equiv 0$

$$\mathbf{c} = (\mathbf{L} + \zeta \sigma^2 \text{diag}(\mathbf{U}\mathbf{1}_C)^{-1})^{-1} (\text{diag}(\mathbf{U}\mathbf{1}_C)^{-1} \mathbf{U}\mathbf{X} - \mathbf{Y})$$

\mathbf{L} Gram 矩阵 $l_{ij} = K(\mathbf{y}_i, \mathbf{y}_j)$

$$\mathbf{T} = \mathcal{T}(\mathbf{Y}) = \mathbf{Y} + \mathbf{L}\mathbf{c}$$

无监督聚类启发的非刚性配准

更新 ν

$$\mathbf{c} = (\mathbf{L} + \zeta \sigma^2 \text{diag}(\mathbf{U}\mathbf{1}_C)^{-1})^{-1} (\text{diag}(\mathbf{U}\mathbf{1}_C)^{-1} \mathbf{U}\mathbf{X} - \mathbf{Y})$$

基于聚类的 Nyström 低秩矩阵逼近

对source 点集进行聚类 获取聚类中心

$$\{\mathbf{z}_i \in \mathbb{R}^n\}_{i=1}^{C'} \quad (C' \ll C)$$

$$O(C^3) \xrightarrow{C' = C^{1/3}} O(C)$$

$$\mathbf{L} \approx \mathbf{E}\mathbf{W}^{-1}\mathbf{E}^T$$

$$\mathbf{E} = [e_{ij}] \in \mathbb{R}^{C \times C'} \quad e_{ij} = K(\mathbf{y}_i, \mathbf{z}_j)$$

$$\mathbf{W} = [w_{ij}] \in \mathbb{R}^{C' \times C'} \quad w_{ij} = K(\mathbf{z}_i, \mathbf{z}_j)$$

无监督聚类启发的非刚性配准

基于聚类的 Nyström 低秩矩阵逼近

$$\mathbf{L} \approx \mathbf{E}\mathbf{W}^{-1}\mathbf{E}^T$$

$$\mathbf{E} = [e_{ij}] \in \mathbb{R}^{C \times C'} \quad e_{ij} = K(\mathbf{y}_i, \mathbf{z}_j)$$

$$\mathbf{W} = [w_{ij}] \in \mathbb{R}^{C' \times C'} \quad w_{ij} = K(\mathbf{z}_i, \mathbf{z}_j)$$

低秩矩阵逼近误差界

Proposition 1. *The low-rank approximation error $\epsilon = \|\mathbf{L} - \mathbf{E}\mathbf{W}^{-1}\mathbf{E}^T\|_F$ in terms of the Laplacian kernel is bounded by*

$$\epsilon \leq 4\sqrt{2}T^{3/2}\gamma\sqrt{C'q} + 2C'\gamma^2Tq\|\mathbf{W}^{-1}\|_F, \quad (11)$$

where $\|\cdot\|_F$ is the matrix Frobenius norm, $T = \max_i |\mathbf{P}_i|$, $q = \sum_{j=1}^C \|\mathbf{y}_j - \mathbf{z}_{c'(j)}\|_2^2$ is the clustering quantization error with $c'(j) = \operatorname{argmin}_{i=1, \dots, C'} \|\mathbf{y}_j - \mathbf{z}_i\|_2$, and γ is the Laplacian kernel bandwidth defined in Eq. (8).

无监督聚类启发的非刚性配准

算法总结

1. 将非刚性点集配准问题建模为聚类过程
2. 变量更新有闭形式解，可直接交替优化
3. 聚类低秩矩阵逼近，严格误差界
4. 和点集嵌入空间维度无关，适用 \mathbb{R}^n

配准

Source

Target

形变

聚类

聚类中心

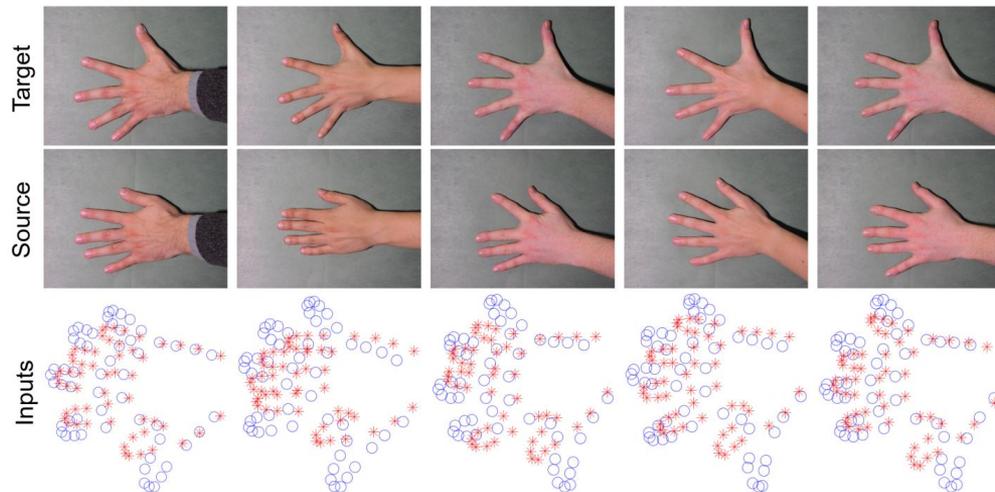
聚类样本

聚类更新

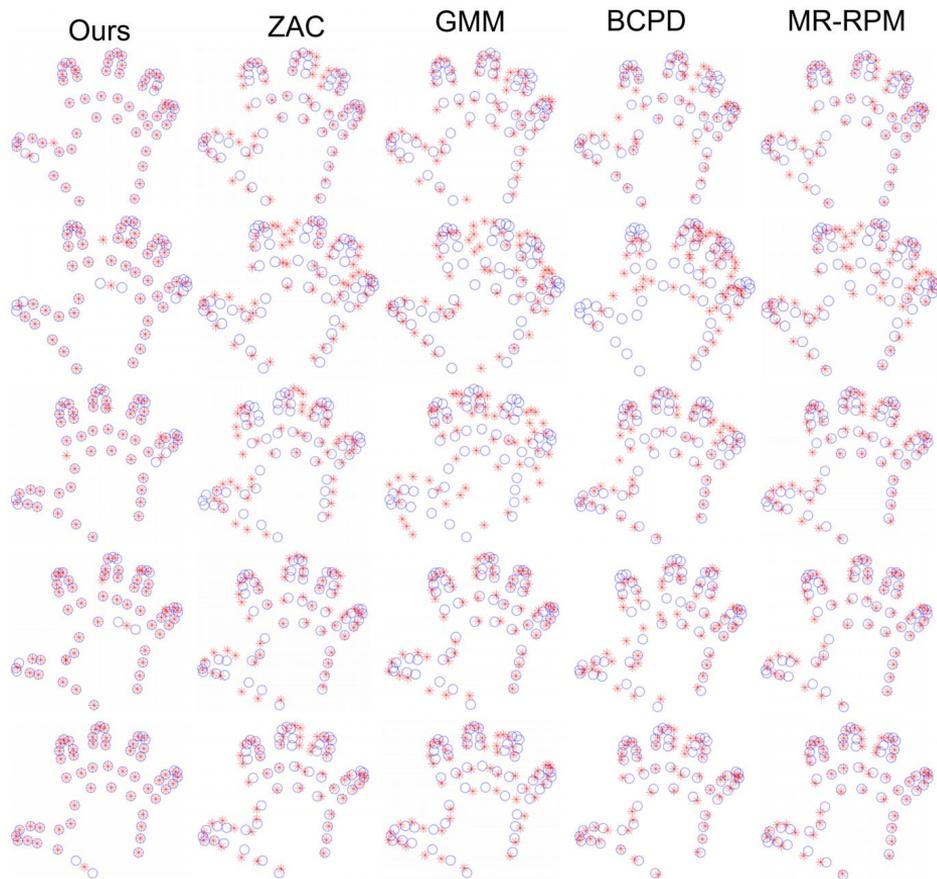
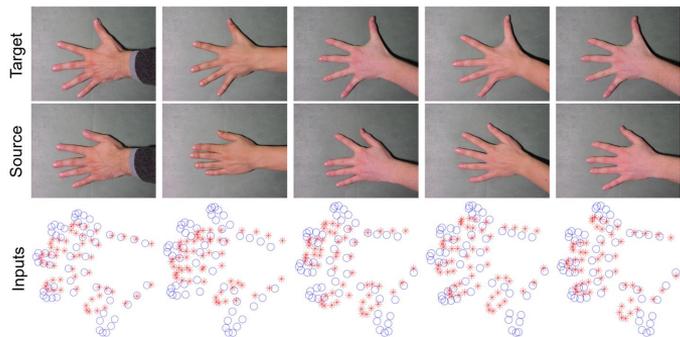
实验

非刚性点集配准——2D

Method	Subject 1	Subject 2	Subject 3	Subject 4	Time (s)
MR-RPM [30]	0.0940	0.0834	0.1028	0.1388	0.2382
BCPD [20]	0.1027	0.1055	0.1080	0.1579	0.6890
GMM [23]	0.0571	0.0547	0.0734	0.0917	0.1140
ZAC [45]	0.4886	0.4566	0.4879	0.4935	0.4254
Ours	0.0383	0.0481	0.0537	0.0879	0.1074



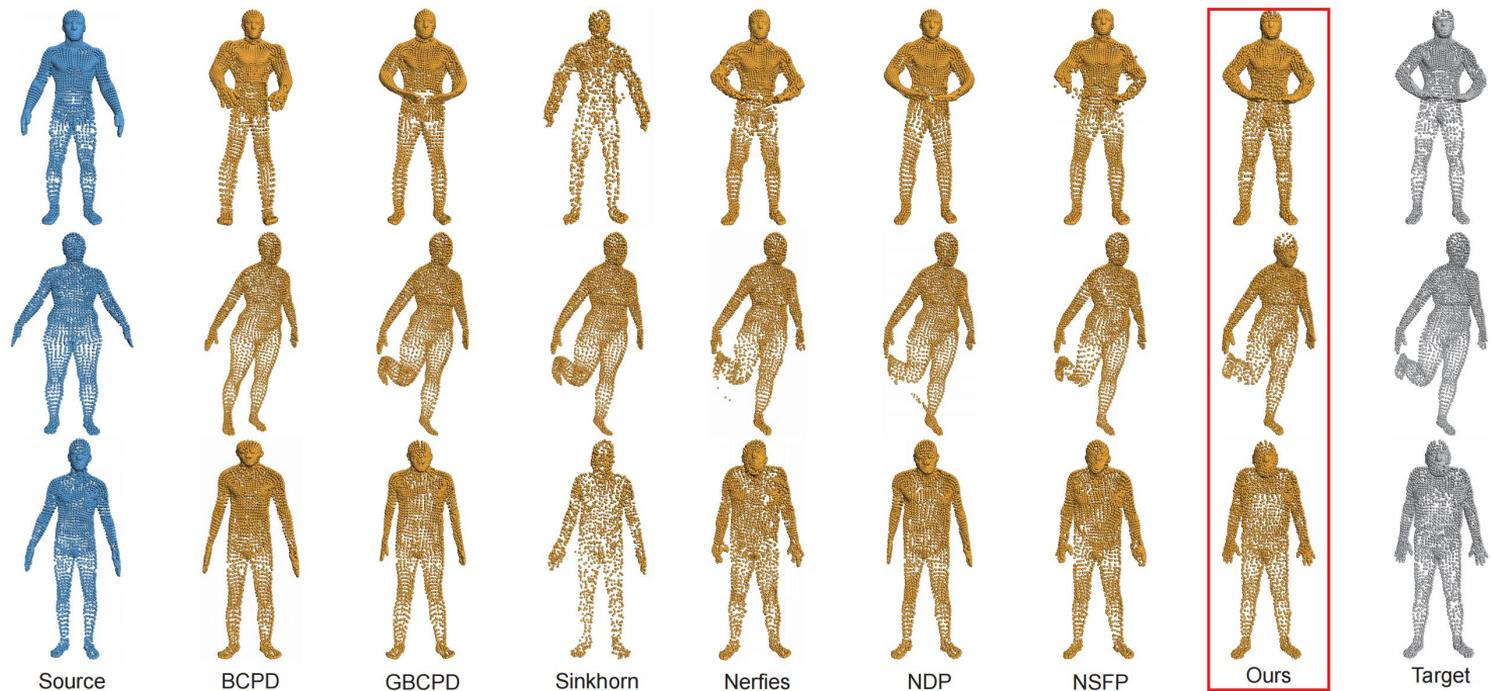
非刚性点集配准——2D



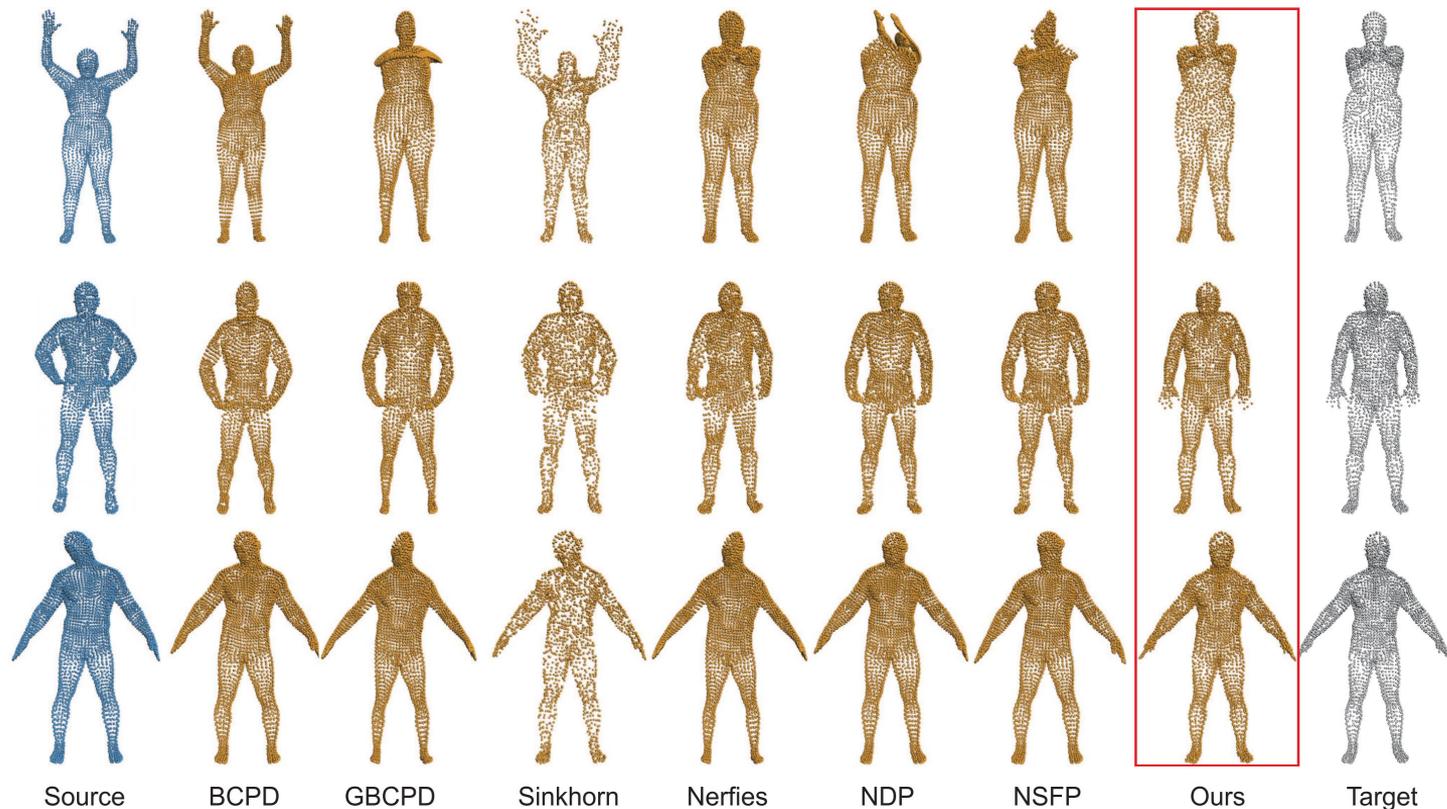
非刚性点集配准——3D

Settings Method	Intra-1	Intra-2	Intra-3	Intra-4	Intra-5	Intra-6	Inter-1	Inter-2	Inter-3	Inter-4	Average
BCPD [20]	0.0913	0.1011	0.0872	0.0577	0.1004	0.0746	0.1196	0.0705	0.0935	0.0923	0.0888
GBCPD [21]	0.0285	0.0212	0.0211	0.0260	0.0244	0.0339	0.0359	0.0340	0.0212	0.0190	0.0265
Fast_RNRR [47]	0.0430	0.0487	0.0397	0.0504	0.0429	0.0391	0.1358	0.0743	0.0477	0.0358	0.0557
AMM_NRR [48]	0.0544	0.0486	0.0400	0.0539	0.0405	0.0393	0.0838	0.0686	0.0422	0.0399	0.0511
Sinkhorn [16]	0.0654	0.0638	0.1372	0.1096	0.0749	0.0821	0.2467	0.0781	0.1400	0.1720	0.1170
Nerfies [35]	0.0120	0.0107	0.0138	0.0129	0.0135	0.0118	0.0121	0.0144	0.0140	0.0140	0.0129
NDP [26]	0.0183	0.0199	0.0192	0.0152	0.0170	0.0149	0.0181	0.0198	0.0164	0.0155	0.0174
NSFP [24]	0.0126	0.0134	0.0132	0.0118	0.0137	0.0142	0.0167	0.0162	0.0148	0.0166	0.0143
Ours	0.0086	0.0089	0.0103	0.0096	0.0089	0.0081	0.0097	0.0099	0.0094	0.0081	0.0092

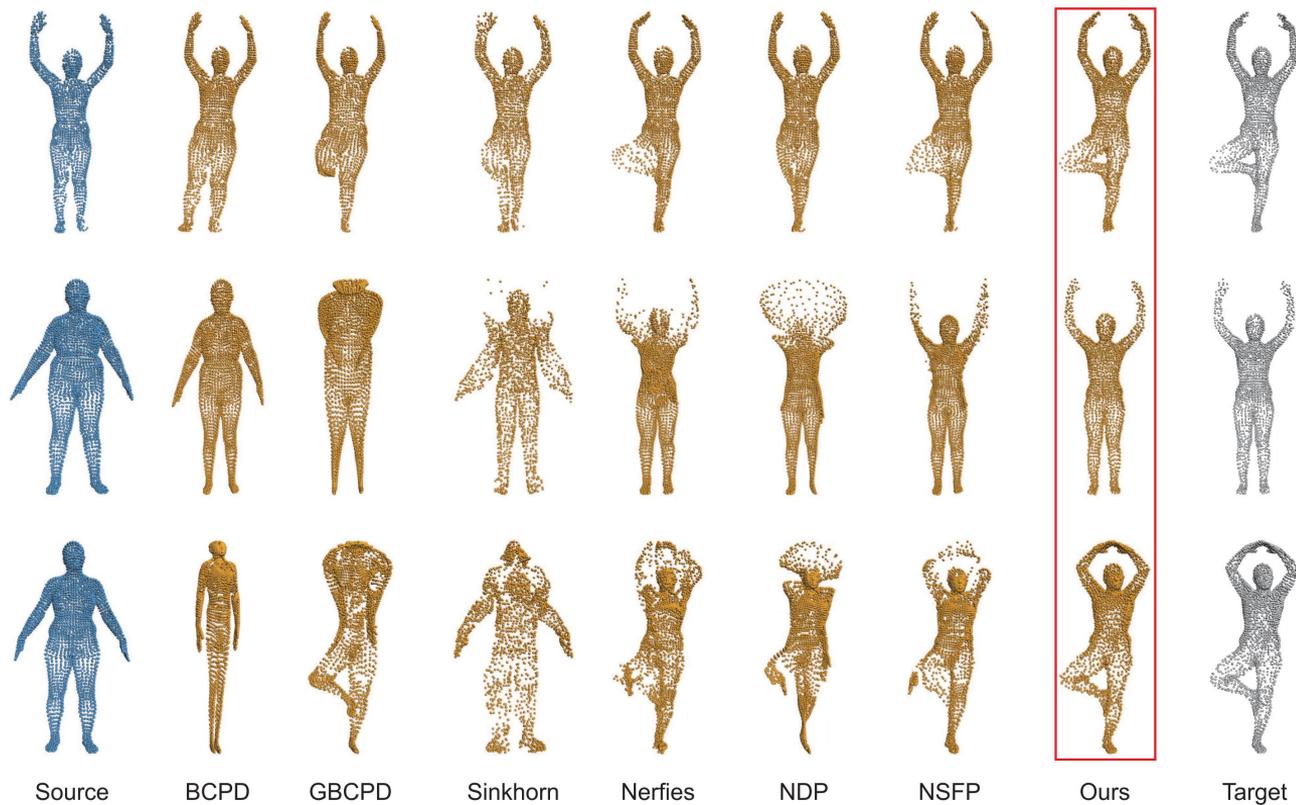
非刚性点集配准——3D



非刚性点集配准——3D



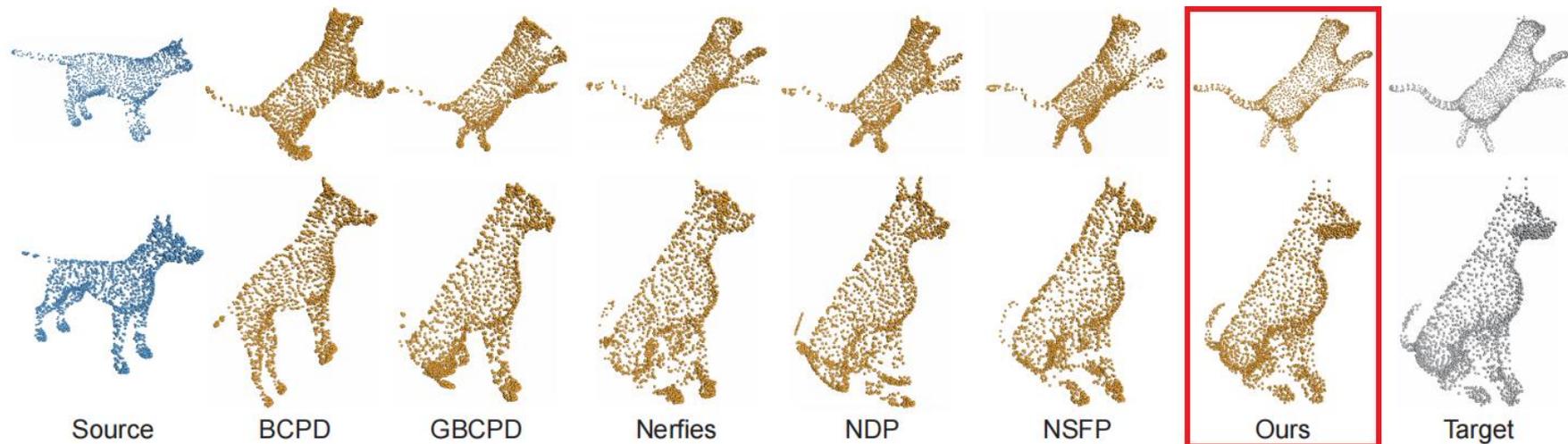
非刚性点集配准——3D



非刚性点集配准——3D

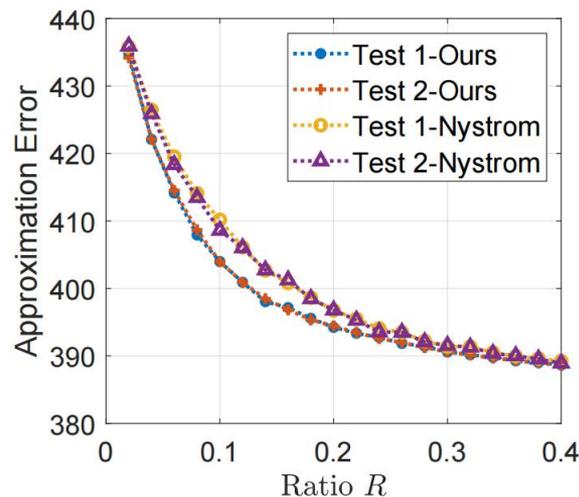
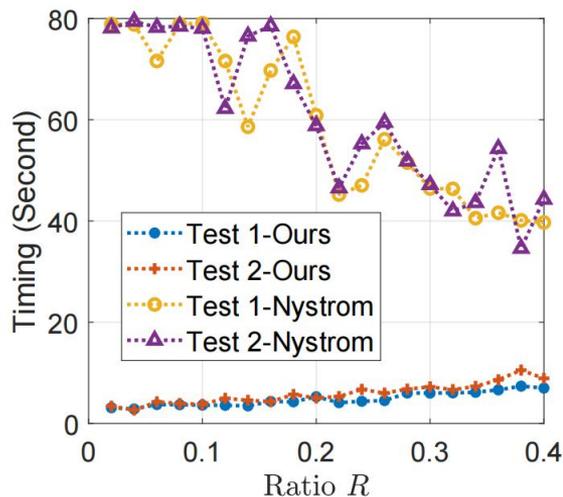
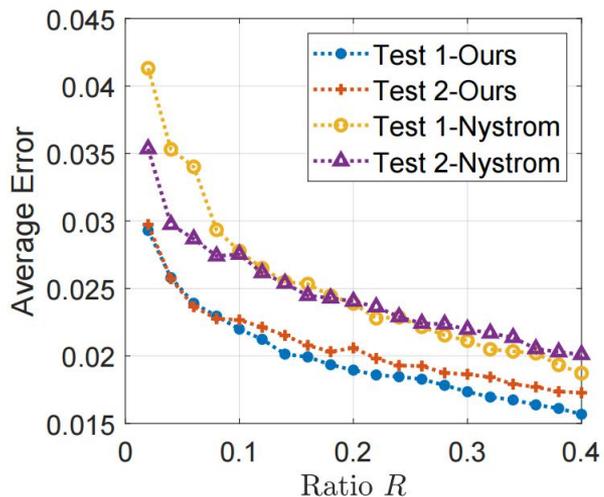
Method	Cat	Centaur	Dog	Gorilla	Average
BCPD [20]	3.9884	8.1017	7.2800	5.6253	5.9935
GBCPD [21]	1.5631	2.9480	1.5300	3.5751	2.6523
Nerfies [35]	3.2704	2.8826	1.3612	2.2809	2.3211
NDP [26]	4.3639	3.4373	3.1285	2.8312	3.2560
NSFP [24]	1.8774	2.6425	1.6734	2.2044	2.0710
Ours	1.3496	1.8125	1.2088	1.6807	1.5247

非刚性点集配准——3D



非刚性点集配准——消融实验

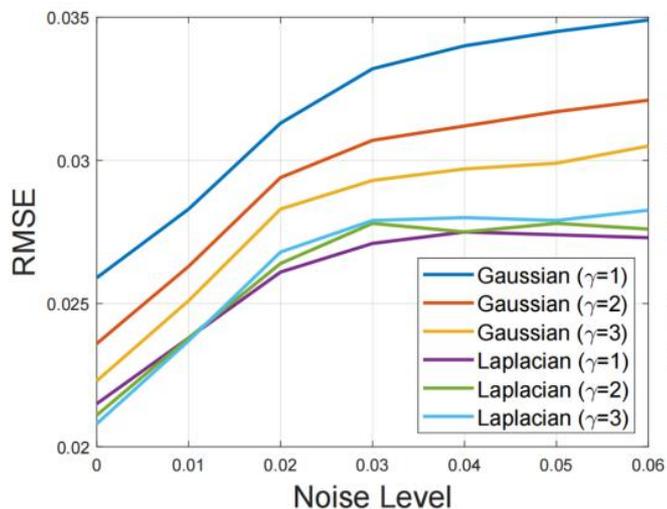
聚类 Nyström VS. 非聚类



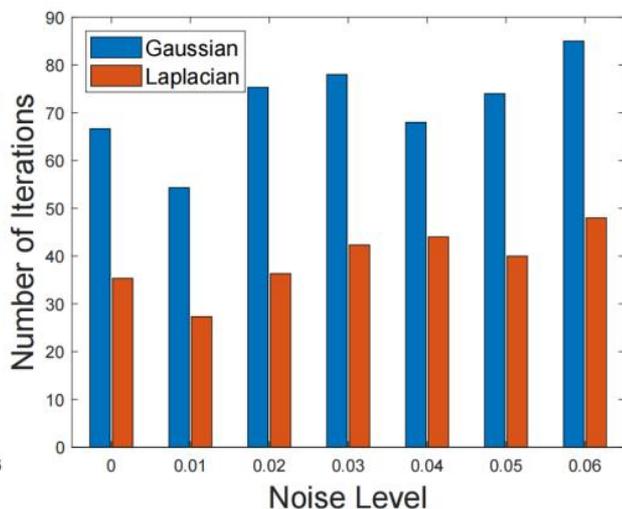
基于聚类的 Nyström 低秩矩阵逼近的配准精度和速度都显著优于非聚类的

非刚性点集配准——消融实验

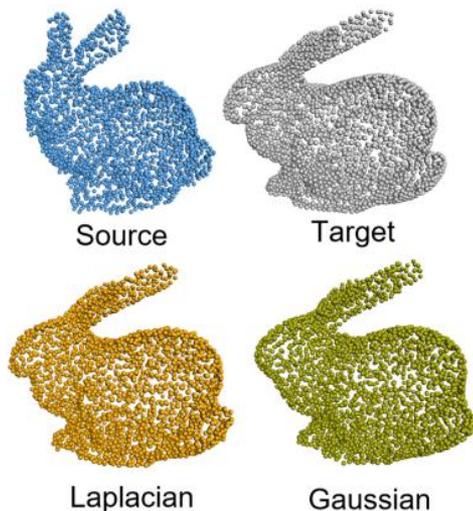
Laplacian VS. Gaussian kernel



(a)



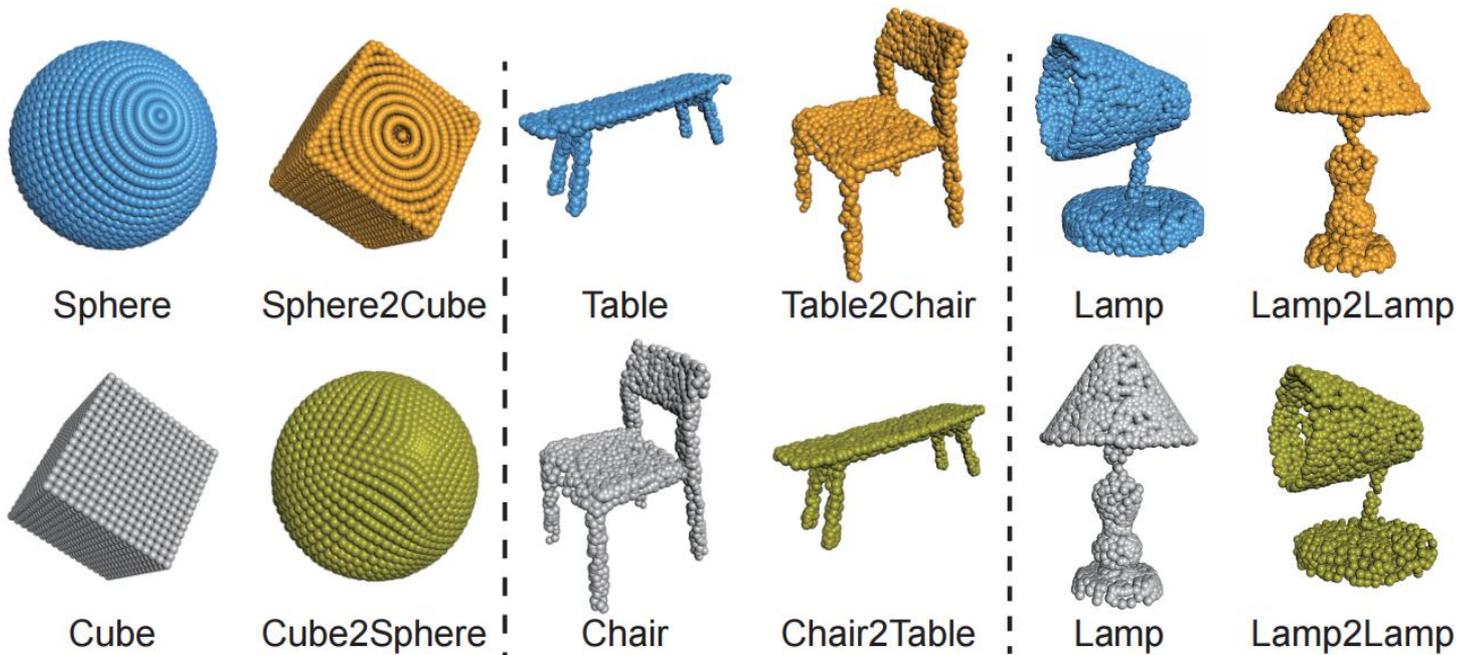
(b)



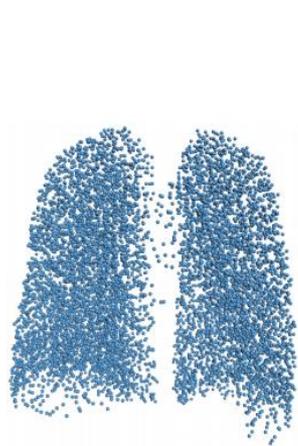
(c)

基于Laplacian kernel的配准精度和收敛速度均显著优于Gaussian kernel

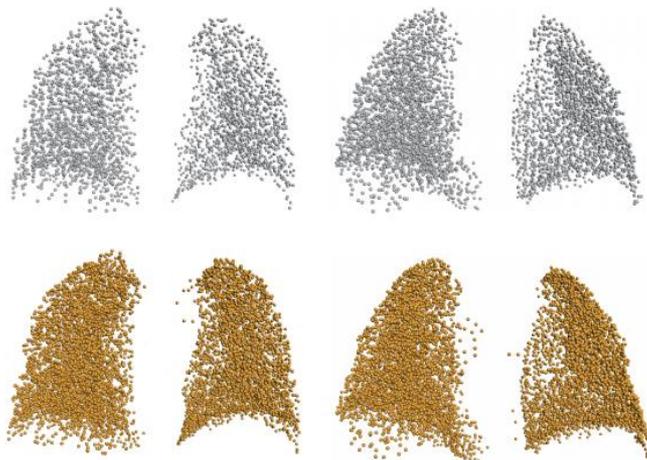
非刚性点集配准——形状迁移



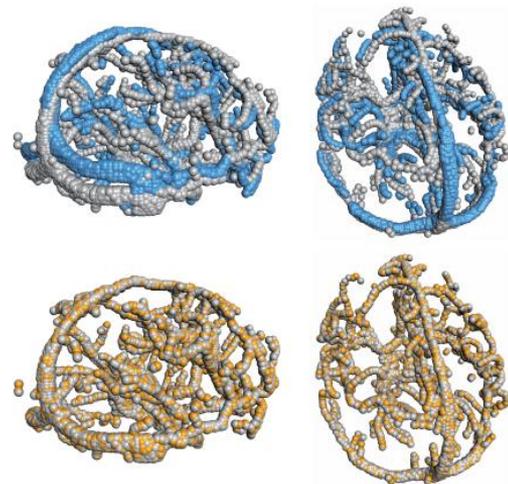
非刚性点集配准——医学数据



Inhale Lung



Exhale Lung



Brain Vessel

展望

非刚性配准——难点

非刚性配准

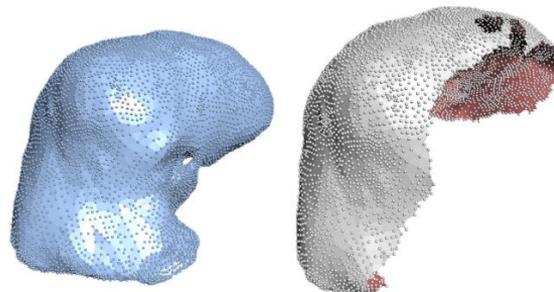
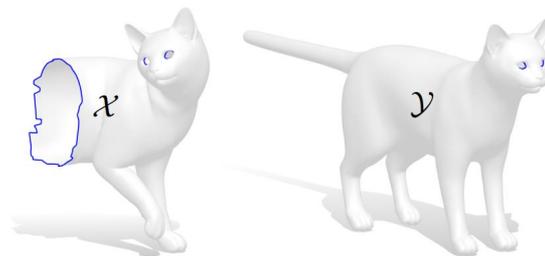
形状遮挡

显著形变

多视角

其他几何表示

.....



术前

术中

遮挡程度增加
无对应部分的形变如何确定？
先验形状补全？

非刚性配准——难点

非刚性配准

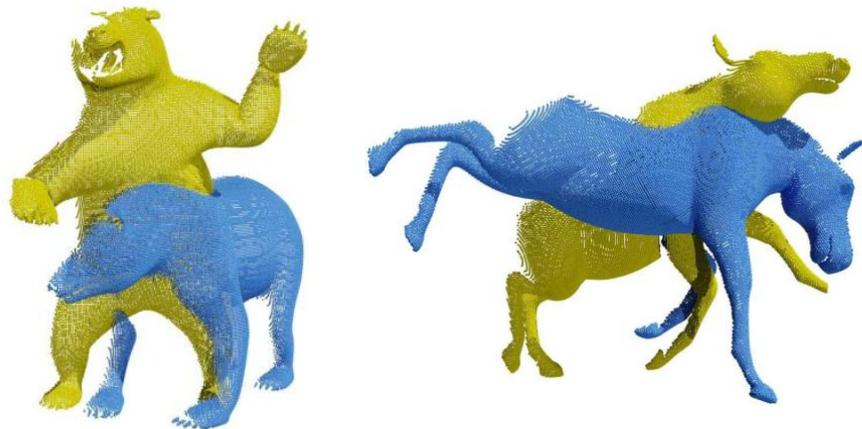
形状遮挡

显著形变

多视角

其他几何表示

.....



通过特征匹配提供初始化

非刚性配准——难点

非刚性配准

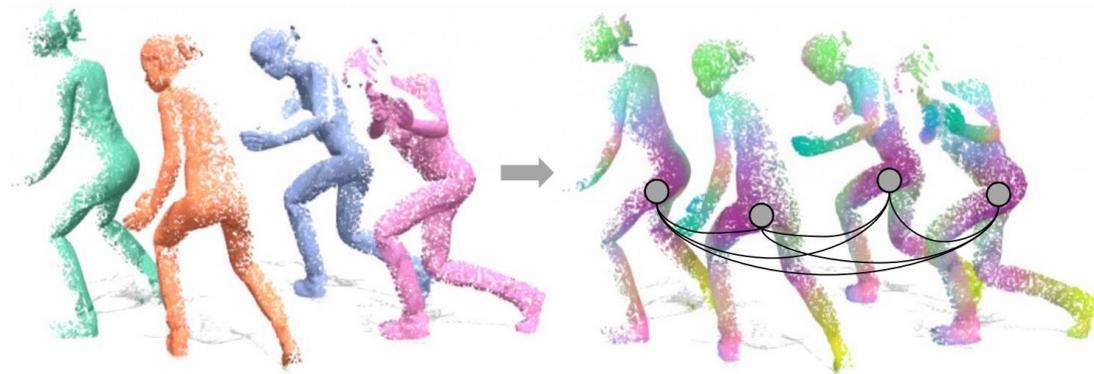
形状遮挡

显著形变

多视角

其他几何表示

.....



如何缓解累积误差

非刚性配准——难点

非刚性配准

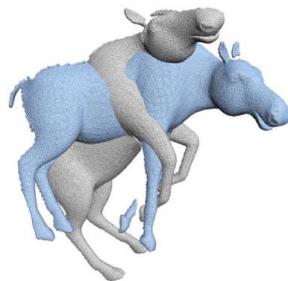
形状遮挡

显著形变

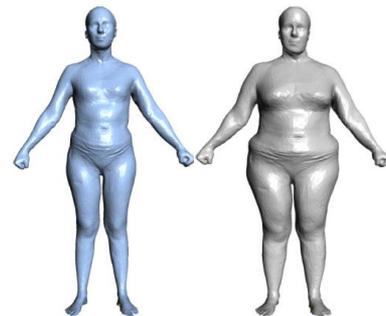
多视角

其他几何表示

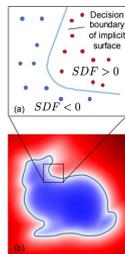
.....



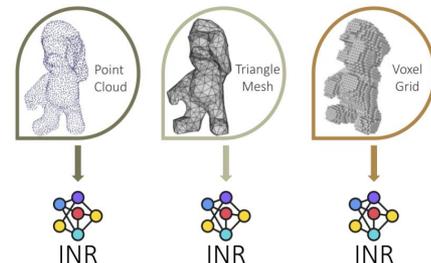
Point cloud



Mesh



SDF



INR

[1] Park et al., DeepSDF: Learning Continuous Signed Distance Functions for Shape Representation, CVPR, 2019

[2] Luigi et al., Deep Learning on Implicit Neural Representations of Shapes, ICLR, 2023

非刚性配准——应用

非刚性配准

NeRF

Gaussian splatting

Image morphing

.....



(a) Capture Process

(b) Input

(c) Nerfie

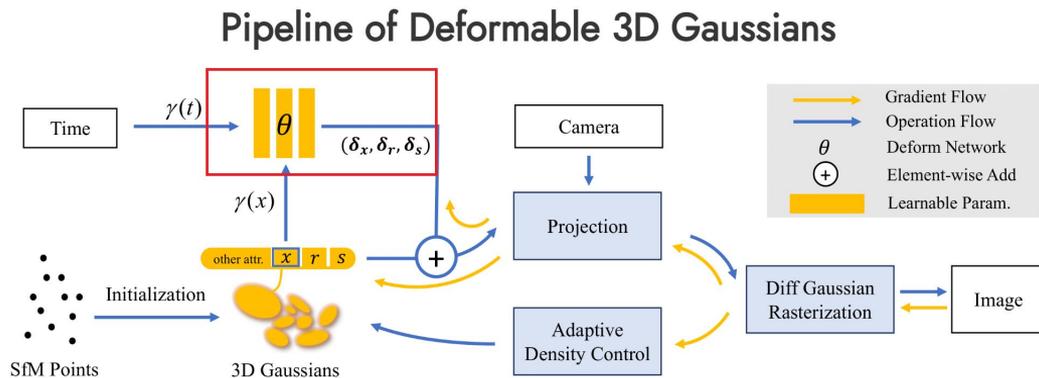
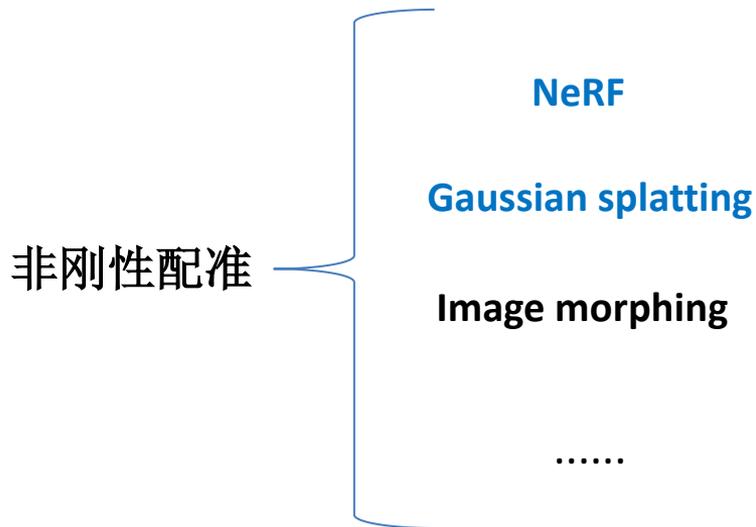
(d) Nerfie Depth



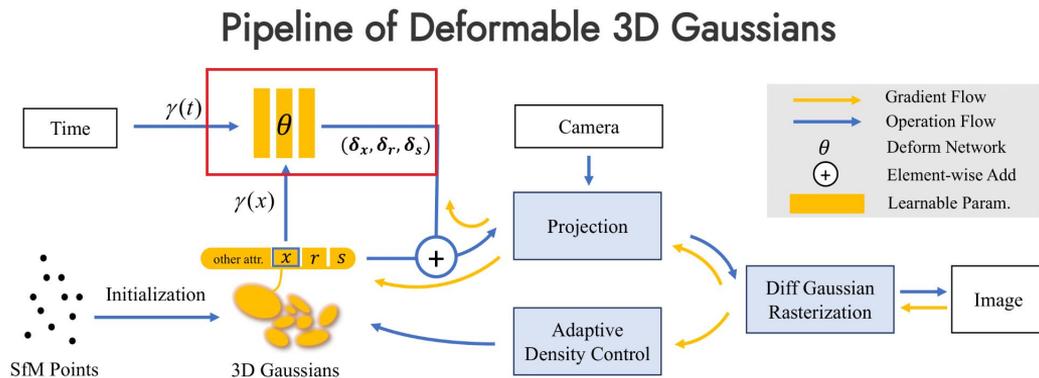
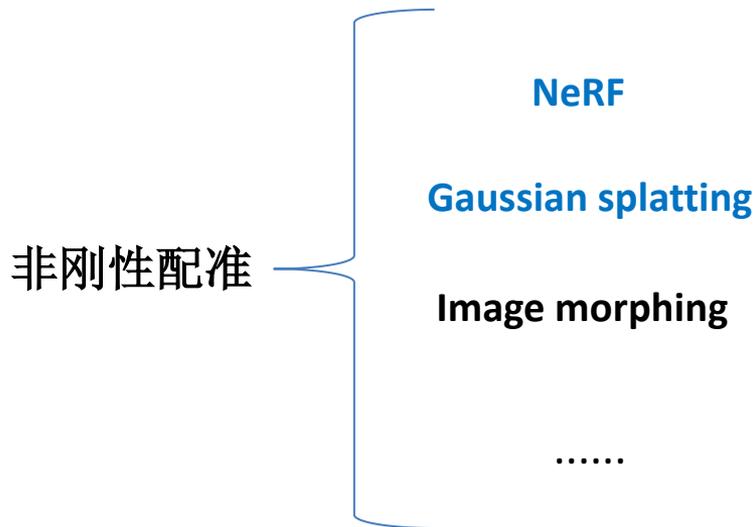
[1] Park et al., Nerfies: Deformable Neural Radiance Fields, ICCV, 2021

[2] Yang et al., Deformable 3D Gaussians for High-Fidelity Monocular Dynamic Scene Reconstruction, CVPR, 2024

非刚性配准——应用



非刚性配准——应用



***THANK YOU FOR YOUR
ATTENTION!***



Code & Project