Multi-Frequency Vector Diffusion Maps

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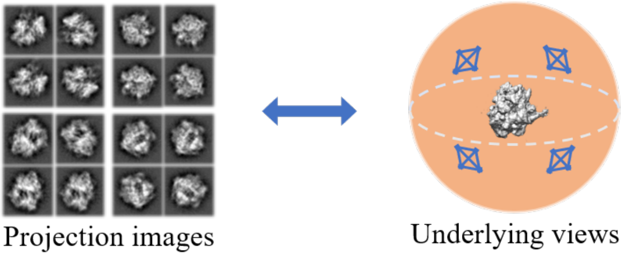
Motivation

Geometry of cryo-electron microscopy single particle images:



Nonlinear dimensionality reduction:

- Locally linear embedding (LLE), ISOMAP, Hessian LLE, Laplacian eigenmaps, Diffusion maps (DM).
- Vector diffusion maps (VDM) generalizes diffusion maps (DM) to define heat kernels for vector fields on the manifold.

Problem setup

- Given a dataset $x_i \in \mathbb{R}^l$ for $i = 1, \ldots, n$:

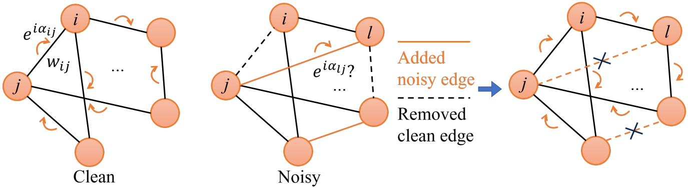
$$\mathcal{G}\text{-invariant distance: } d_{ij} = \min_{g \in \mathcal{G}} \|x_i - g \cdot x_j\|,$$

$$\text{optimal alignment: } g_{ij} = \arg\min_{g \in \mathcal{G}} \|x_i - g \cdot x_j\|.$$

- Data points lie on or close to a low-dimensional manifold $\mathcal{X}$ and we define $\mathcal{M} = \mathcal{X}/\mathcal{G}$.
- Define **neighborhood graph based on the invariant distance**: $G = (V, E)$ by $(i, j) \in E \Leftrightarrow d_{ij} \leq \epsilon$, with the associated alignment $g_{ij} \in \mathcal{G}$.
- In cryo-EM single particle images example, $\mathcal{G} = \mathrm{SO}(2)$, which is the in-plane rotation within each image.

Multi-frequency vector diffusion maps

- **Challenge**: Noisy data induces **inaccurate low-dimensional embedding**.
- **Goal**: Robustly learn the nonlinear geometrical structure of data from noisy measurements to improve nearest neighbor search and alignment.
- **Our work**: **Multi-frequency vector diffusion maps (MFVDM)**.
  1. Extend VDM by using **multiple irreducible representation**.
  2. Achieve more accurate nearest neighbor identification and alignment.



Multi-frequency vector diffusion maps

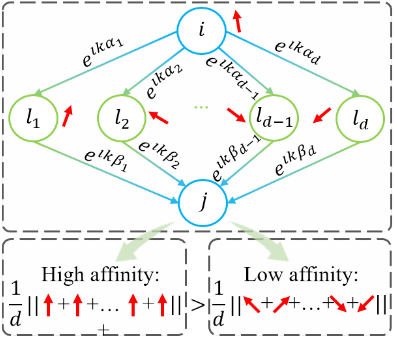
- **Intuition**: For neighbor points in $\mathcal{M}$, the alignments should have **cycle consistency across multiple irreducible representations**, e.g., for neighbor nodes i, j and l, **for each** $\boldsymbol{k} \in \mathbb{Z}$,

$$\boxed{k(\alpha_{ij} + \alpha_{jl} + \alpha_{li}) \approx 0 \bmod 2\pi.}$$

- MFVDM builds a series of weight matrices W_k for $k = 1, \ldots, k_{\max}$:

$$W_k(i,j) = \begin{cases} w_{ij} e^{\imath k \alpha_{ij}} & (i,j) \in E, \\ 0 & \text{otherwise,} \end{cases}$$

Degree matrix $D(i,i) = \sum_{j:(i,j)\in E} w_{ij}$.



VDM for each frequency k

- Define the affinity matrix S_k for frequency k:

$$S_k = D^{-1/2} W_k D^{-1/2} = \sum_{l=1}^{n} \lambda_l^{(k)} u_l^{(k)}(i) \overline{u_l^{(k)}(j)}$$

with $\lambda_1^{(k)} \geq \lambda_2^{(k)} \geq \ldots \geq \lambda_n^{(k)}$.

- The affinity between i and j is given as $|S_k^{2t}(i,j)|$.
- VDM mapping for frequency k:

$$\hat{V}_t^{(k)} : i \mapsto \left(\left(\lambda_l^{(k)} \lambda_r^{(k)} \right)^t \langle u_l^{(k)}(i), u_r^{(k)}(i) \rangle \right)_{l,r=1}^{m_k}.$$

We call this **frequency-k-VDM**, $m_k \ll n$ is a truncation parameter.

Multi-frequency vector diffusion maps

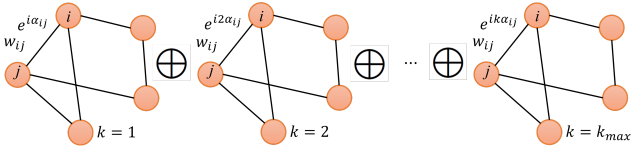
- **Multi-frequency vector diffusion maps**: Concatenate $\hat{V}_t^{(k)}$ for $k = 1, \dots, k_{\max}$:

$$\boxed{\hat{V}_t(i) : i \mapsto \left(\hat{V}_t^{(1)}(i); \hat{V}_t^{(2)}(i); \dots; \hat{V}_t^{(k_{\max})}(i) \right).}$$

- **Multi-frequency vector diffusion distance**:

$$d^2_{\mathrm{MFVDM},t}(i,j) = \left\| \frac{\hat{V}_t(i)}{\|\hat{V}_t(i)\|} - \frac{\hat{V}_t(j)}{\|\hat{V}_t(j)\|} \right\|_2^2 .$$

- Using multiple irreducible representation leads to a **highly robust measure of neighbor points on $\mathcal{M}$**.



Nearest neighbor identification & alignment

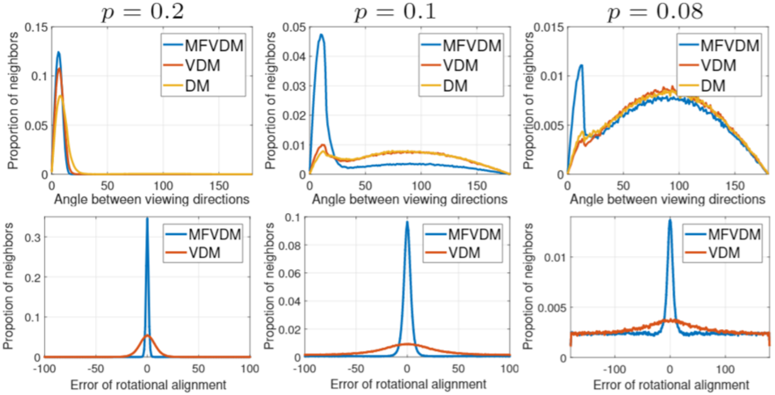
- Identify nearest neighbors based on $d^2_{\mathrm{MFVDM},t}(i,j)$.
- Experiments: simulate $n = 10^4$ on a 2-sphere, the group transformation $\mathcal{G} = \mathrm{SO}(2)$. We connect each point with its 150 neighbors, optimal alignment has been pre-computed.
- Noise is added following the **random rewiring model**:

$$(i,j) \in E = \begin{cases} (i,j) & \text{with probability } p \\ (i,j) \to (i,l), \alpha_{il} \in \mathrm{Unif}[0,2\pi) & \text{with probability } 1-p \end{cases}$$

Random rewiring

Nearest neighbor identification & rotational alignment

- Histograms of nearest neighbor identification accuracy (The histogram with more points close to 0 is better) and rotational alignment errors.
- MFVDM is very robust to noise.



Thank you!

- Poster #266: Wed Jun 12th 06:30 – 09:00 PM @ Pacific Ballroom.
- Our paper is available at: http://proceedings.mlr.press/v97/fan19a/fan19a.pdf