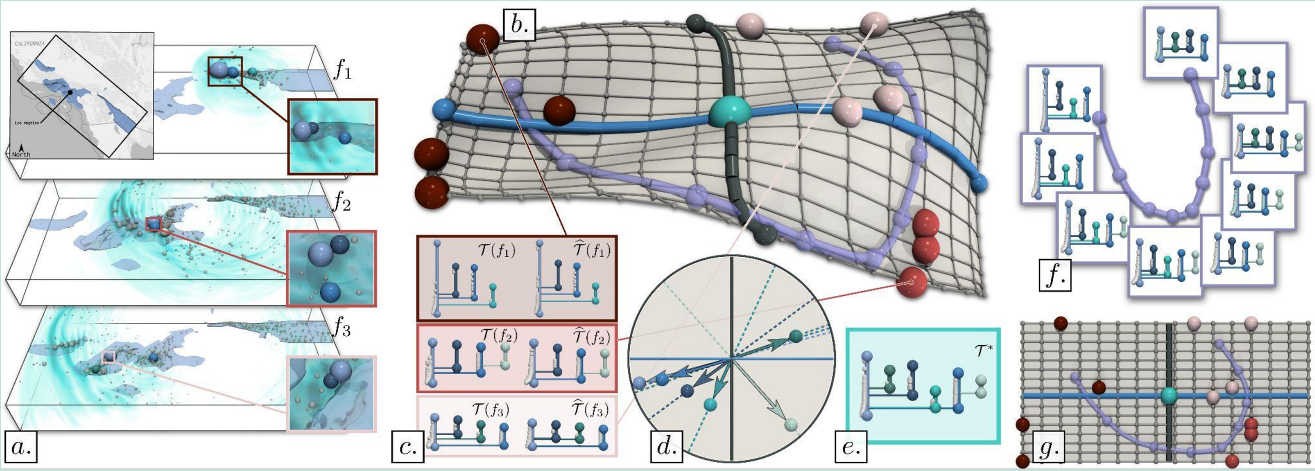
Principal Geodesic Analysis of Merge Trees (and Persistence Diagrams)

Of M. Pont, J. Vidal and J. Tierny



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MATHÉMATIQUES
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Ensemble datasets

Challenge : Several datasets for one phenomenon

-> Each dataset is called an ensemble member

-> Each ensemble member is represented by a Merge Tree

Merge Tree and BDT

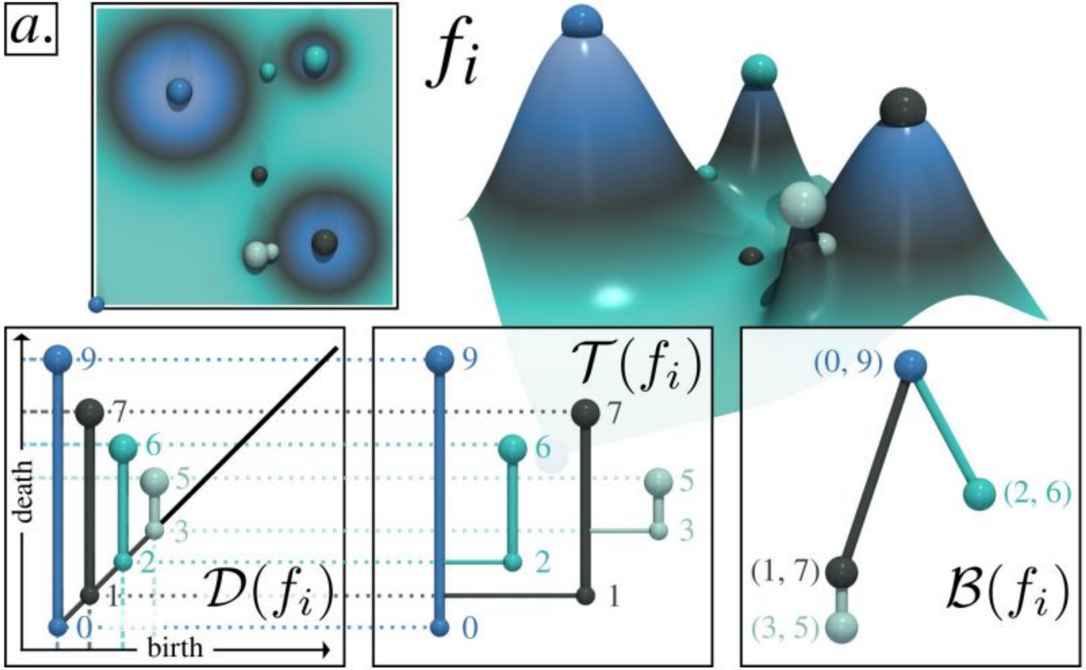
We consider a manifold and a Piecewise Linear scalar function on it

$$f : \mathcal{M} \to \mathbb{R}$$

Merge tree = M/~ where p1~p2 if f(p1) = f(p2) and p1,p2 in the same connected component of the sublevel (or superlevel) set of f at f(p1).

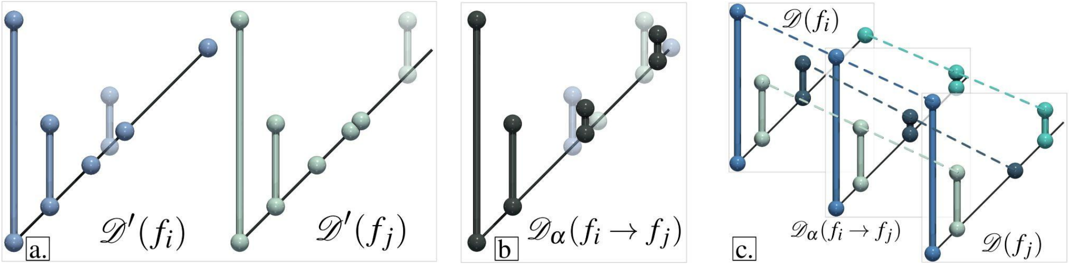
Branch Decomposition Tree (BDT) : A tree with nodes as the persistence branches and edges between adjacent branches.

Merge Tree and BDT



Wasserstein distance on persistence diagrams

- Partial assignment between
  - Off-diagonal points
    - Subset P_i
    - Complement $\overline{P_i}$
  - Bijection $\phi : P_i \to P_j$
  - Partial assignment $(\phi, \overline{P_i}, \overline{P_j}) \in \Phi$



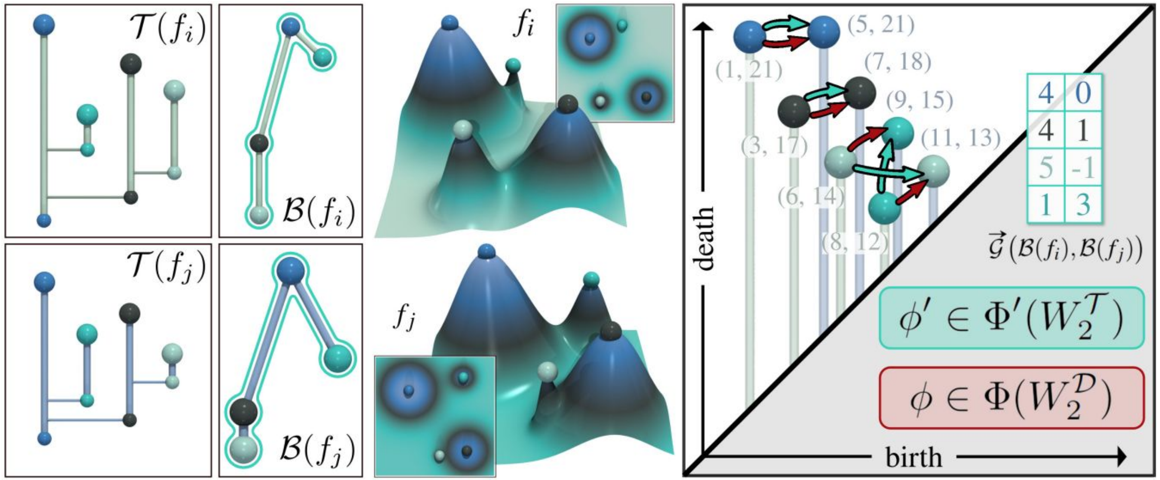
$$W_q(\mathcal{D}(f_i), \mathcal{D}(f_j)) = \min_{(\phi, \overline{P_i}, \overline{P_j}) \in \Phi} \Big(\sum_{p_i \in P_i} d_q(p_i, \phi(p_i))^q + \sum_{p_i \in \overline{P_i}} d_q(p_i, \Delta(p_i))^q + \sum_{p_j \in \overline{P_j}} d_q(\Delta(p_j), p_j)^q \Big)^{1/q}$$

Wasserstein distance on Merge trees

- Same, for q = 2 but $\phi : P_i \to P_j$ must be a partial rooted isomorphism

Partial isomorphism : Operates only on a subset P_i - no difference

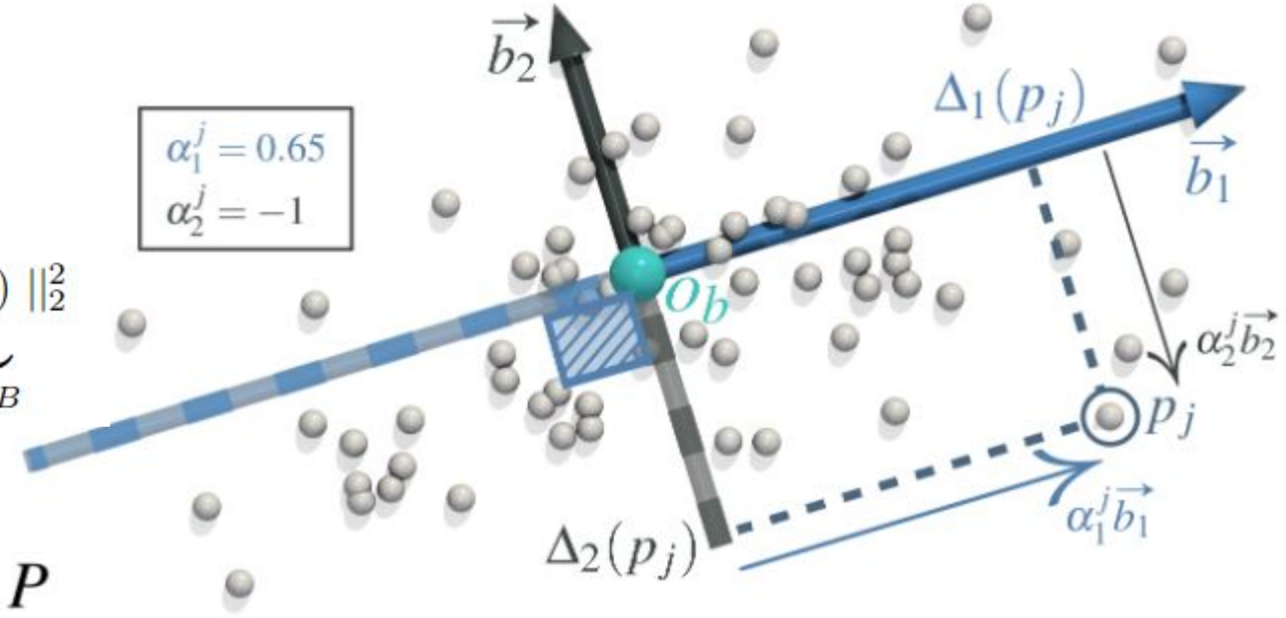
Rooted isomorphism : Conserves adjacency relationship.



Recall PCA in R^d

$$P = \{p_1, \ldots, p_N\}, p_j \in \mathbb{R}^d, \forall j$$
$$B = \{v_1, \ldots, v_q\}, v_i \cdot v_j = 0, \forall i \neq j$$

$$E_{L_2}(B) = \sum_{j=1}^{N} ||p_j - \underbrace{(\mathbf{o} + \sum_{i=1}^{q} \alpha_i^j v_i)}_{\text{Proj. of } p_j \text{ onto } B}||_2^2$$



From PCA to MT-PGA

A **geodesic** is a shortest path between two MT $\mathcal{G}(\mathcal{E},\mathcal{E}') = \underset{\phi' \in \Phi'}{\operatorname{argmin}} W_q^{\mathcal{T}}(\mathcal{E},\mathcal{E}')$

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Geodesic dot product:

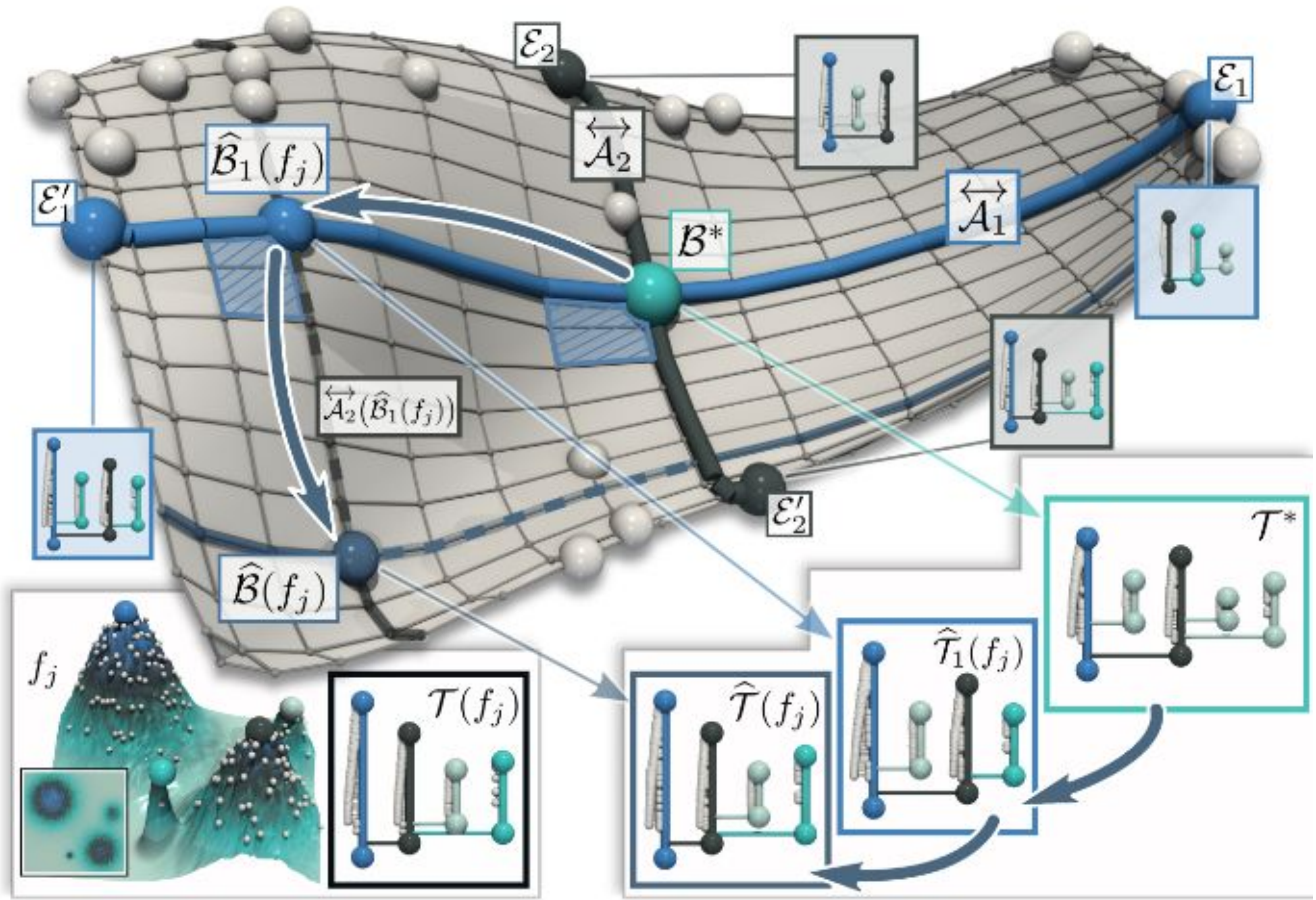
- Share extremity point
- Cartesian dot product in $\mathbb{R}^{2\times|\mathcal{E}|}$

Orthogonal → $\mathcal{G}(\mathcal{E},\mathcal{E}') \cdot \mathcal{G}(\mathcal{E},\mathcal{E}'') = 0$

Collinear→ $\mathcal{G}(\mathcal{E},\mathcal{E}') = \lambda \mathcal{G}(\mathcal{E},\mathcal{E}'')$

Geodesic axis is a pair of negatively collinear geodesics through the origin $\mathcal{E}_o$ → It's a geodesic and defines a direction vector $\mathcal{V}_i = \mathcal{G}(\mathcal{E}_i,\mathcal{E}_i')$ Between the extremities

From PCA to MT-PGA



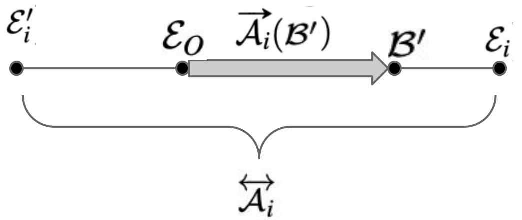
From PCA to MT-PGA

- BDT($\mathcal{B}$) geodesic axis ($\overleftrightarrow{\mathcal{A}_i}$) projection

$$\mathcal{B}_{\overleftrightarrow{\mathcal{A}_i}} = \underset{\mathcal{B}' \in \overleftrightarrow{\mathcal{A}_i}}{\arg\min} \left(W_2^{\mathcal{T}} \left(\mathcal{B}, \mathcal{B}' \right) \right)$$

- BDT ($\mathcal{B}' \in \overleftrightarrow{\mathcal{A}_i}$) geodesic axis arc-length parametrization $\overrightarrow{\mathcal{G}_i'} = \overrightarrow{\mathcal{G}}(\mathcal{E}_O, \mathcal{E}_i')$ $\overrightarrow{\mathcal{G}_i} = \overrightarrow{\mathcal{G}}(\mathcal{E}_O, \mathcal{E}_i)$

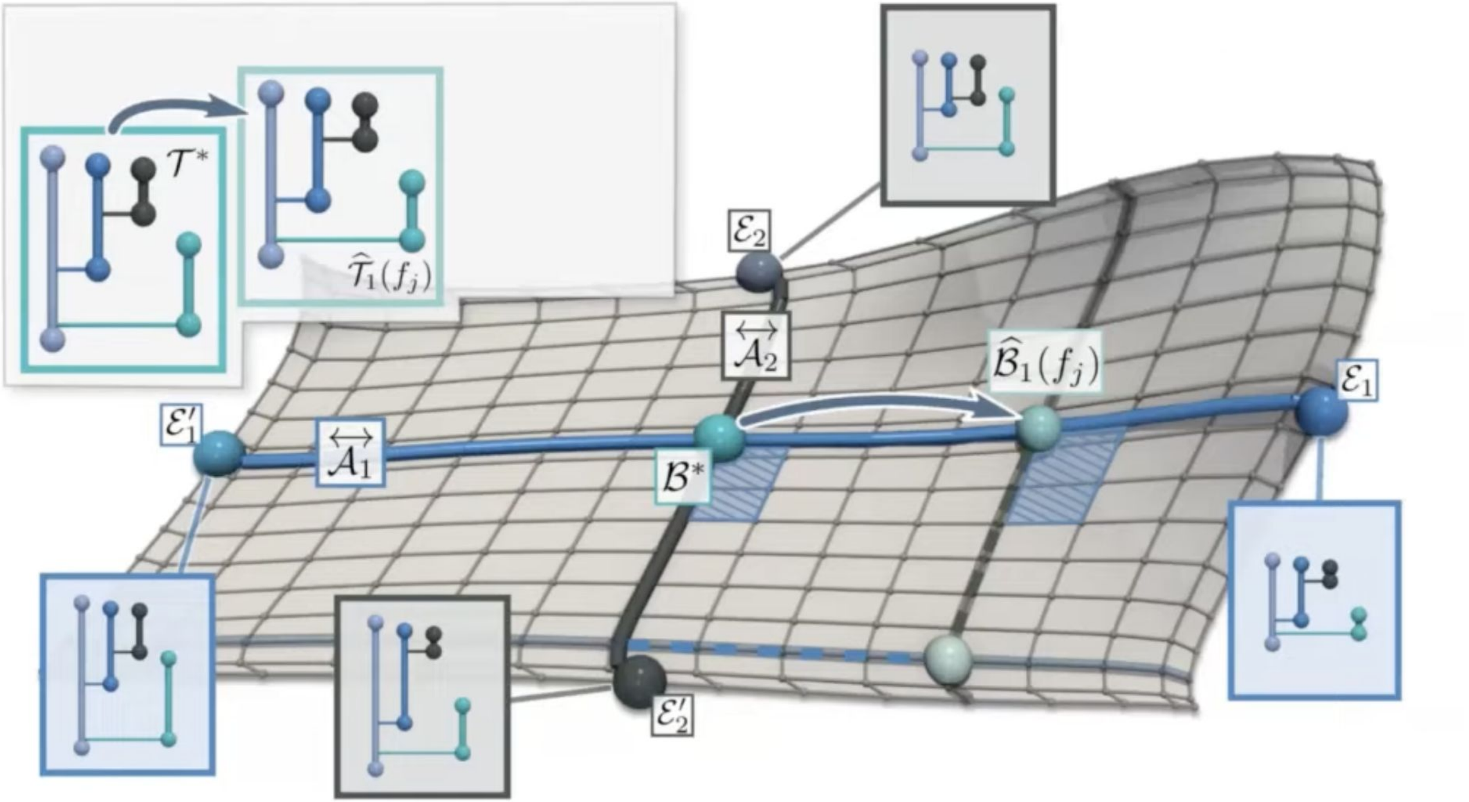
$$\mathcal{B}' = \mathcal{E}_O + \overrightarrow{\mathcal{A}_i}(\mathcal{B}') = \mathcal{E}_O + \alpha_i \times \overrightarrow{\mathcal{G}_i} + (1 - \alpha_i) \times \overrightarrow{\mathcal{G}_i'}.$$



- BDT($\mathcal{B}$) geodesic axis ($\overleftrightarrow{\mathcal{A}_i}$) projection

$$\mathcal{B}_{\overleftrightarrow{\mathcal{A}_i}} = \underset{\mathcal{B}' \in \overleftrightarrow{\mathcal{A}_i}}{\arg\min} \left(W_2^{\mathcal{T}} \left(\mathcal{B}, \mathcal{E}_O + \overrightarrow{\mathcal{A}_i}(\mathcal{B}') \right) \right)$$

- BDT axis translation: $\overleftrightarrow{\mathcal{A}}_j(\mathcal{B}) = ((\mathcal{B}, \mathcal{B} + \overrightarrow{\mathcal{G}_j}), (\mathcal{B}, \mathcal{B} + \overrightarrow{\mathcal{G}'_j}))$



From PCA to MT-PGA

- **BDT geodesic orthogonal basis**

  Orthogonal basis of d' geodesic axes $B_{\mathbb{B}} = \{\overleftrightarrow{\mathcal{A}_1}, \overleftrightarrow{\mathcal{A}_2}, \dots, \overleftrightarrow{\mathcal{A}_{d'}}\}$ with origine $\mathcal{E}_O$

  Project an arbitrary BDT $\mathcal{B}$ on $\overleftrightarrow{\mathcal{A}_1}$: $\widehat{\mathcal{B}}_1 = \mathcal{B}_{\overleftrightarrow{\mathcal{A}_1}} = \mathcal{B}_{\overleftrightarrow{\mathcal{A}_1}(\mathcal{E}_O)}$

  Recursively: $\widehat{\mathcal{B}}_{d'} = \mathcal{B}_{\overleftrightarrow{\mathcal{A}_{d'}}(\widehat{\mathcal{B}}_{d'-1})} \Longrightarrow \widehat{\mathcal{B}}_{d'} = \mathcal{E}_O + \sum_{i=1}^{d'} \overrightarrow{\mathcal{A}_i}(\widehat{\mathcal{B}}_i)$

- **MT-PGA formulation: distance to the constructed basis of BDT**

  $\mathcal{B}^*$: Wasserstein barycenter

$$\boxed{E_{W_2^{\mathcal{T}}}(B_{\mathbb{B}}) = \sum_{j=1}^{N} W_2^{\mathcal{T}}\left(\mathcal{B}(f_j), \mathcal{B}^* + \sum_{i=1}^{d'} \overrightarrow{\mathcal{A}_i}(\widehat{\mathcal{B}}_i(f_j))\right)^2}$$

Algorithm

Finding an orthogonal basis of principal geodesics in the Wasserstein metric space of MTs

⇔

Constrained optimization problem

$$\min_{B_{\mathbb{B}} = \{\overleftrightarrow{\mathcal{A}_1}, \overleftrightarrow{\mathcal{A}_2}, \dots, \overleftrightarrow{\mathcal{A}_{2\times|\mathcal{B}^*|}}\}} \quad E_{W_2^{\mathcal{T}}}(B_{\mathbb{B}}) = \sum_{j=1}^{N} W_2^{\mathcal{T}}\left(\mathcal{B}(f_j), \mathcal{B}^* + \sum_{i=1}^{d'} \overrightarrow{\mathcal{A}_i}(\widehat{\mathcal{B}}_i(f_j))\right)^2$$

subject to
- geodesics
- negative collinearity
- orthogonality

Algorithm

- For d’ in {1, …, d_max}
  - While $E_{W_2^{\mathcal{T}}}(B_{\mathbb{B}})$ decreases
    - Find A_d’ such that it minimizes $E_{W_2^{\mathcal{T}}}(B_{\mathbb{B}})$
    - enforce the 3 constraints on A_d’

As constraint enforcements are not necessarily compatible together -> while loop until convergence:

while $\overleftrightarrow{\mathcal{A}_{d'}}$ evolves **do**

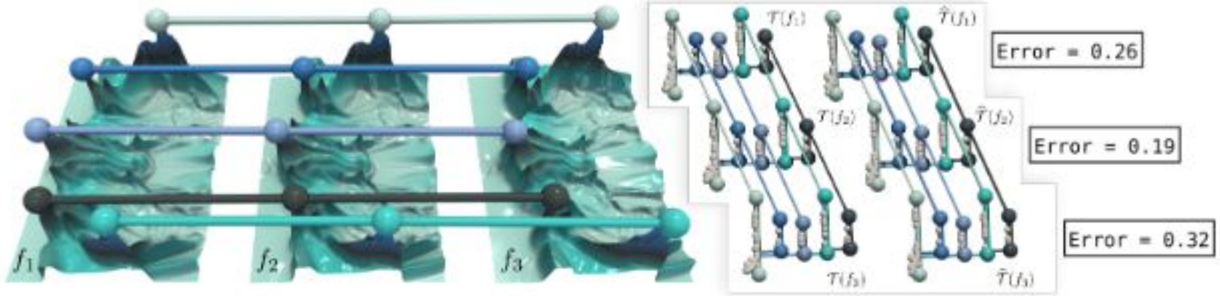
$\overleftrightarrow{\mathcal{A}_{d'}} \leftarrow \text{EnforceGeodesics}(\mathcal{B}^*, \overleftrightarrow{\mathcal{A}_{d'}});$

$\overleftrightarrow{\mathcal{A}_{d'}} \leftarrow \text{EnforceNegativeCollinearity}(\overleftrightarrow{\mathcal{A}_{d'}});$

$\overleftrightarrow{\mathcal{A}_{d'}} \leftarrow \text{EnforceOrthogonality}(B_{\mathbb{B}}, \overleftrightarrow{\mathcal{A}_{d'}});$

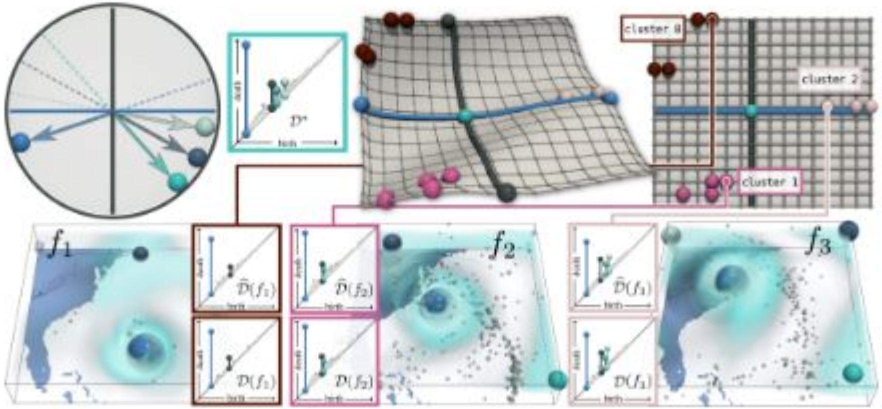
Applications

1. Data reduction → Lossy compression



2. Dimensionality reduction

3. Clustering



Thank you!