



EucApprox - Euclidean Embedding of Data Using Local Distances

Dimitris Arabadjis

Department of Statistics & Actuarial – Financial Mathematics
IDEALab

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Approximate the optimal Euclidean embedding functionally, using only local distance data and local operators

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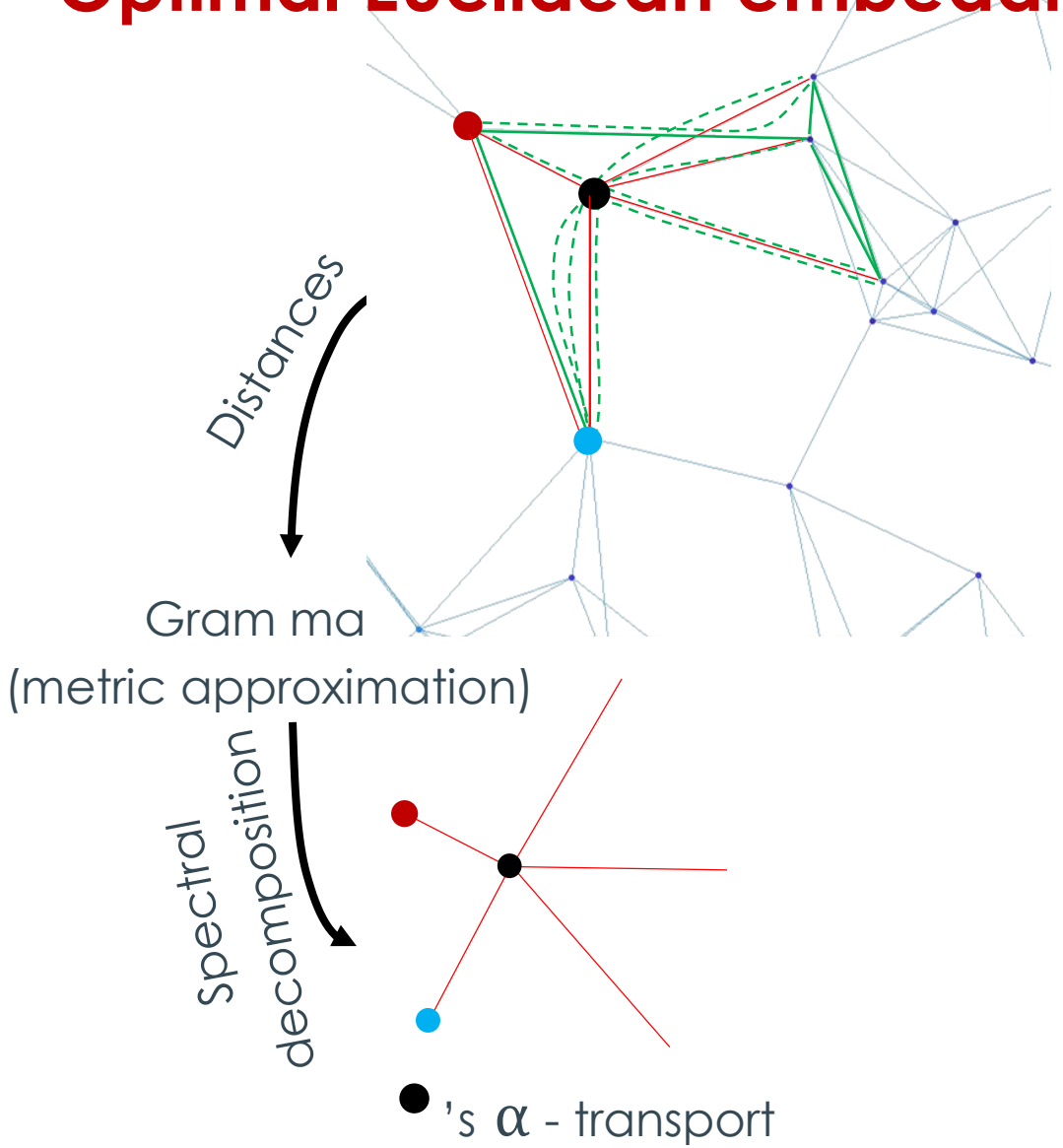
EucApprox	✓	✓	Sparse	Sparse / iterative	Functional

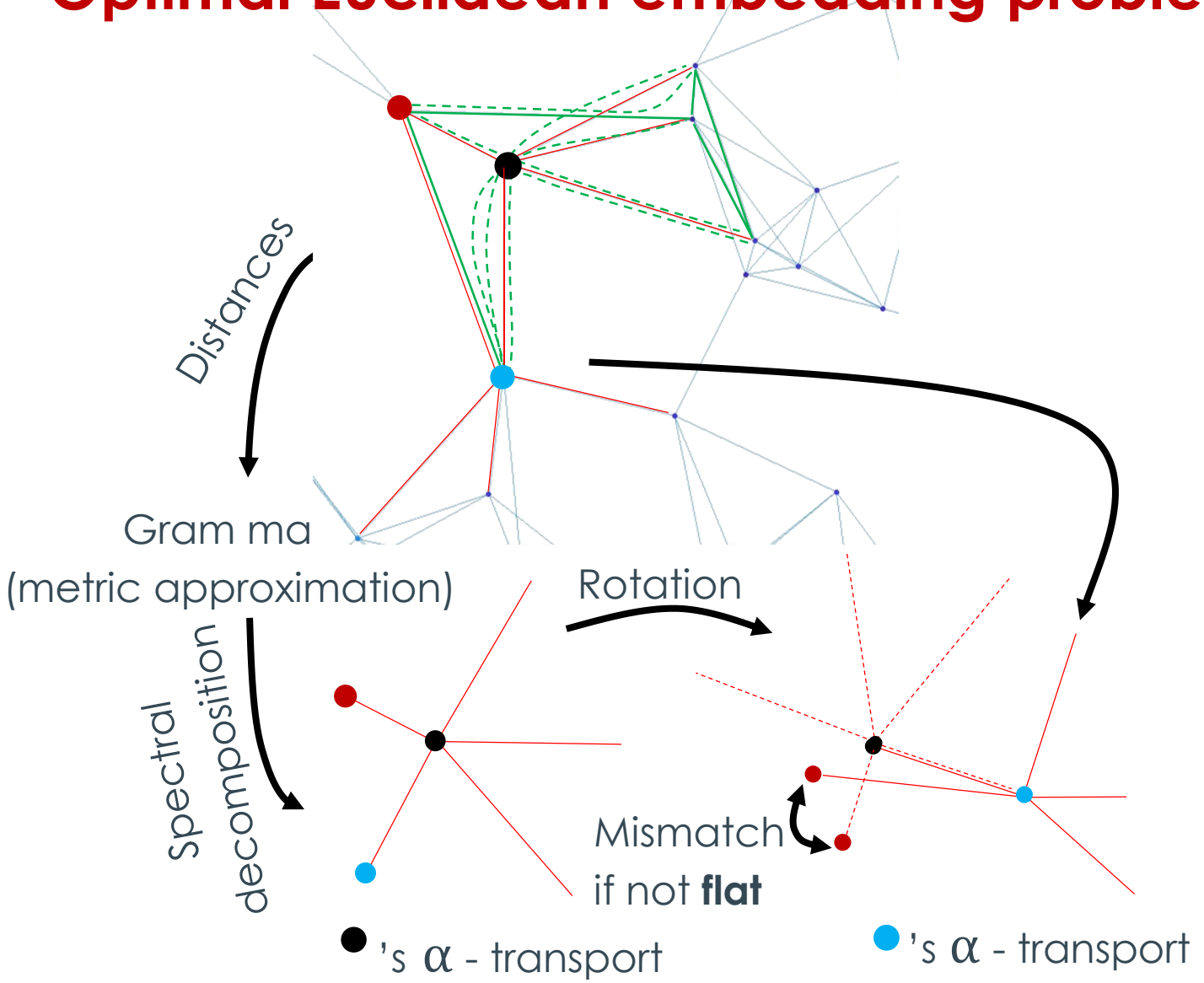
Optimal Euclidean embedding problem



Metric trivializing directions α: Infinitesimal transports that turn the metric into the identity matrix (spectral decomposition of the metric).

Neighbors
Neighborhood's subgraph
Shortest paths

Optimal Euclidean embedding problem



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Only flat manifolds allow to isometrically deform α into integrable entities

Neighbors
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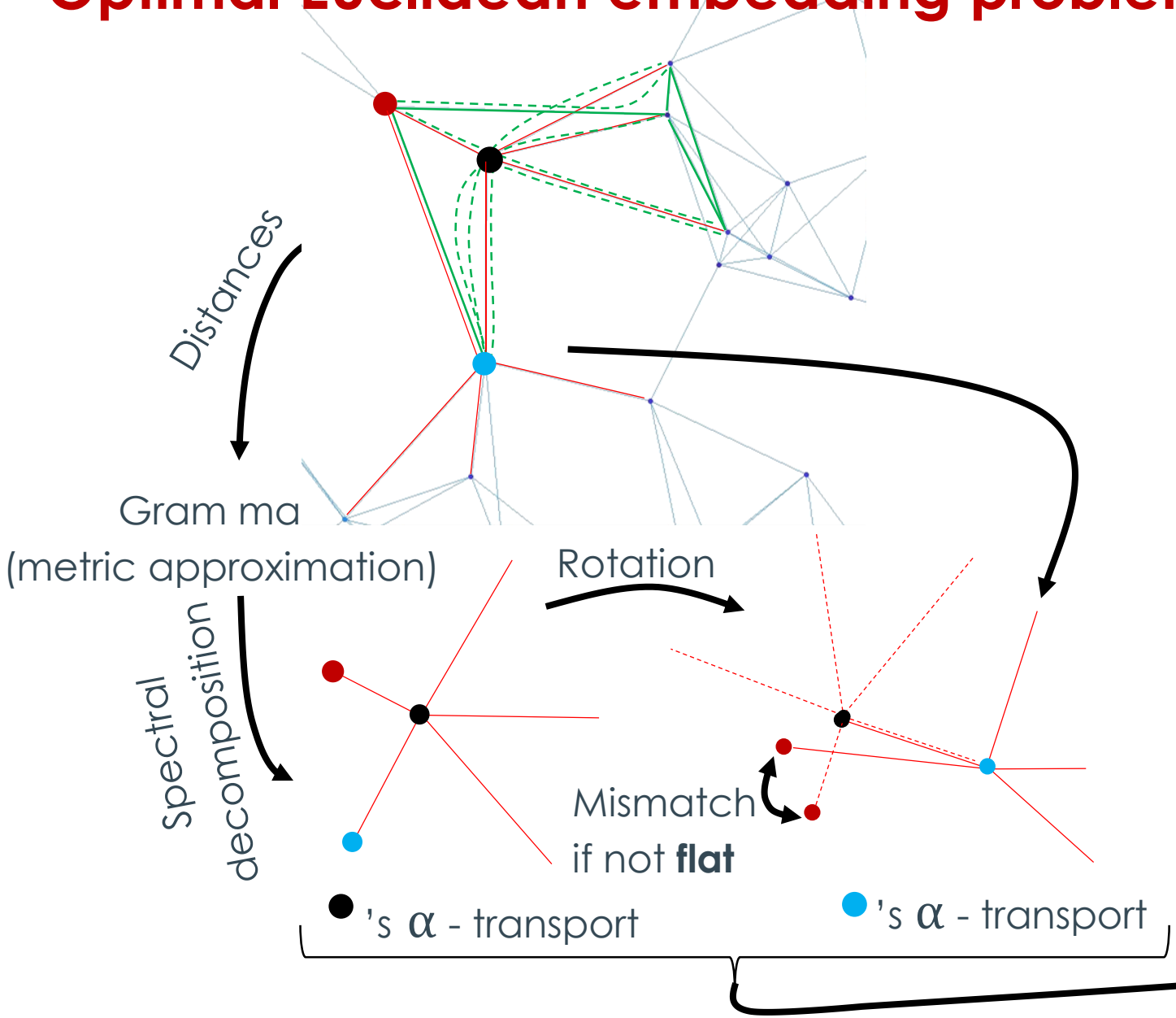
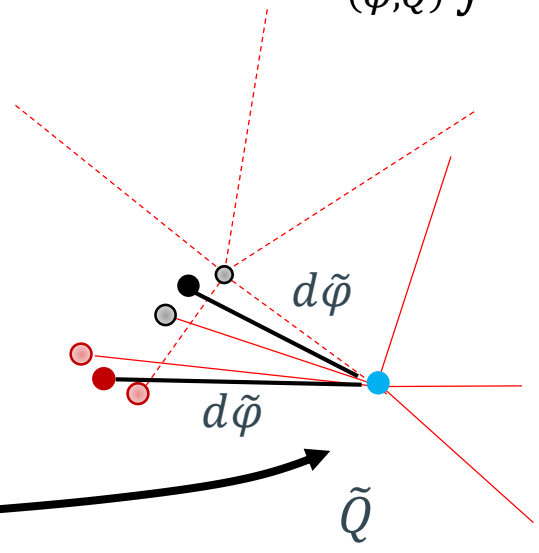
Optimal Euclidean embedding problem



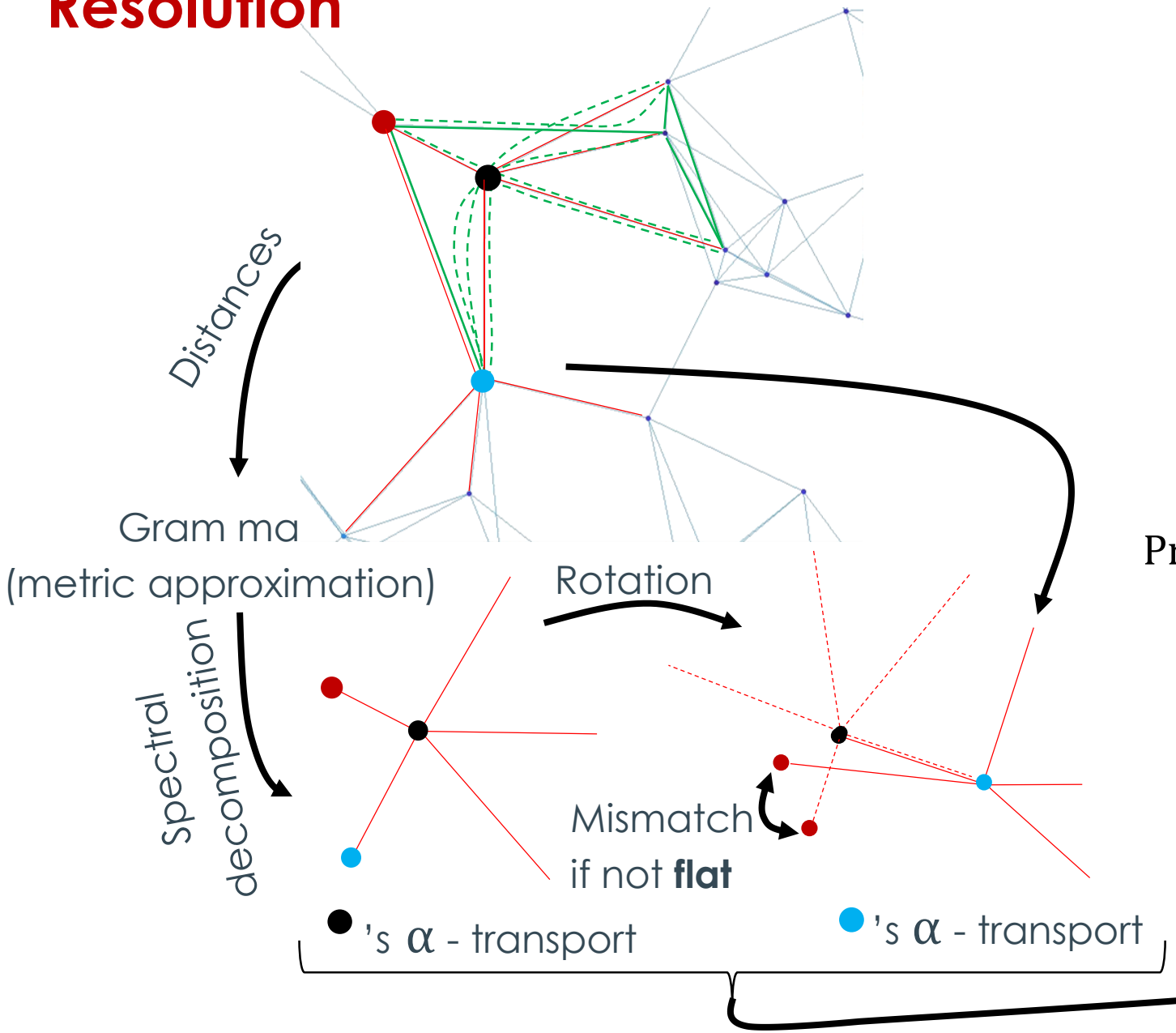
Core idea: Determine the closest integrable entities to the isometries of α.

n – dimensional optimal Euclidean embedding: Find **functions** $\tilde{\varphi} \in \mathbb{R}^N$ and $\tilde{Q} \in O(N)$ so that

$$(\tilde{\varphi}, \tilde{Q}) = \arg\min_{(\varphi,Q)} \int \|d\varphi - \alpha Q\|^2$$



Resolution



Euler-Lagrange equations :

$$\Delta\tilde{\varphi} = \mathrm{div}\left(\alpha\tilde{Q}\right), \qquad \iota_{\partial\Omega}(d\tilde{\varphi}) = \iota_{\partial\Omega}\left(\alpha\tilde{Q}\right)$$

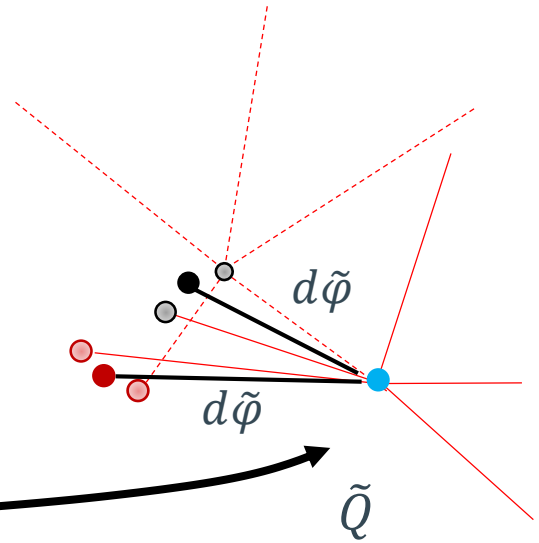
$$\tilde{Q} = \mathrm{Procrustes}(d\tilde{\varphi}, \alpha)$$

Δ – Laplacian

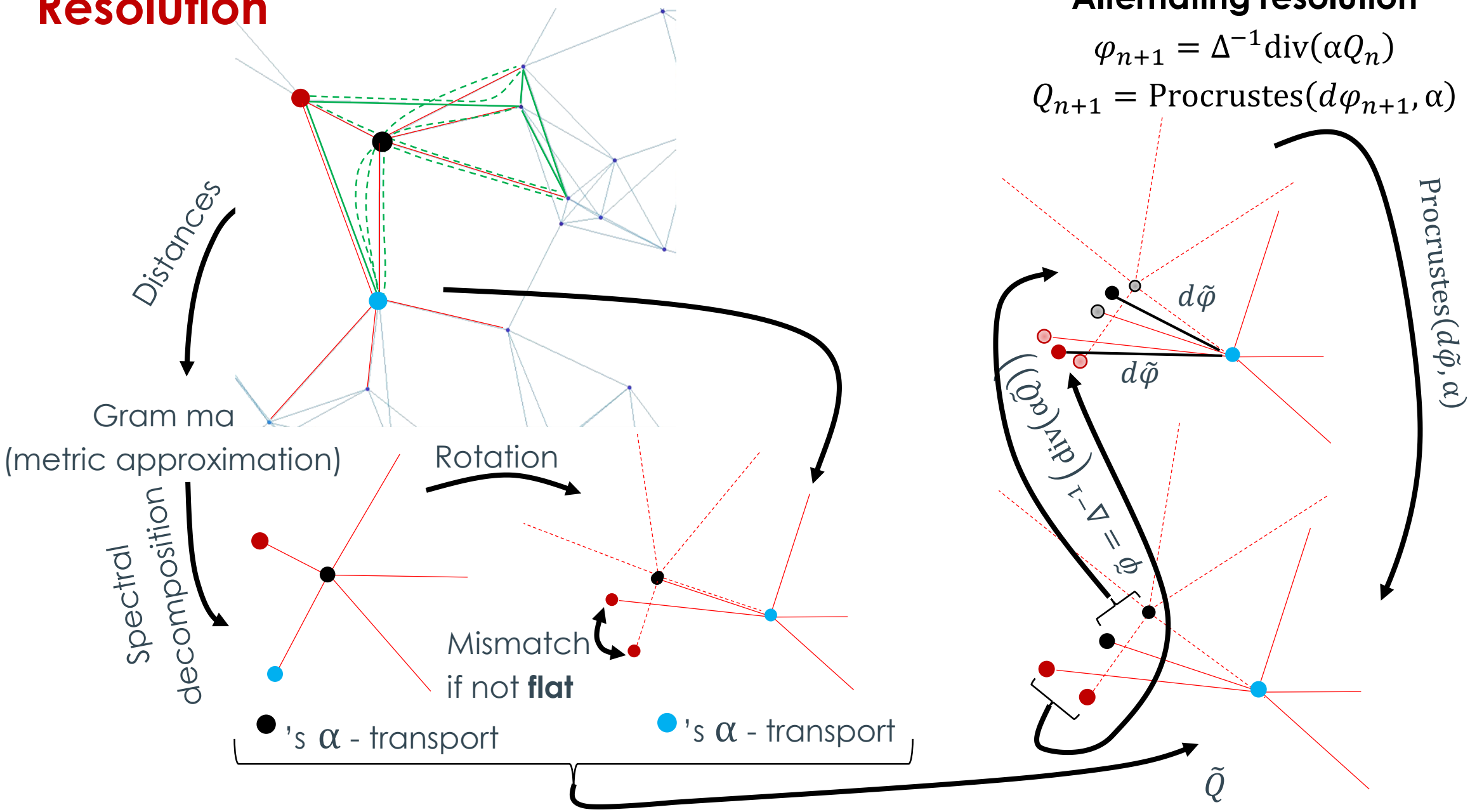
div – divergence

$\iota_{\partial\Omega}(\cdot)$ - inner product with the manifold's boundary normal

$\mathrm{Procrustes}$ – orthogonal Procrustes alignment



Resolution



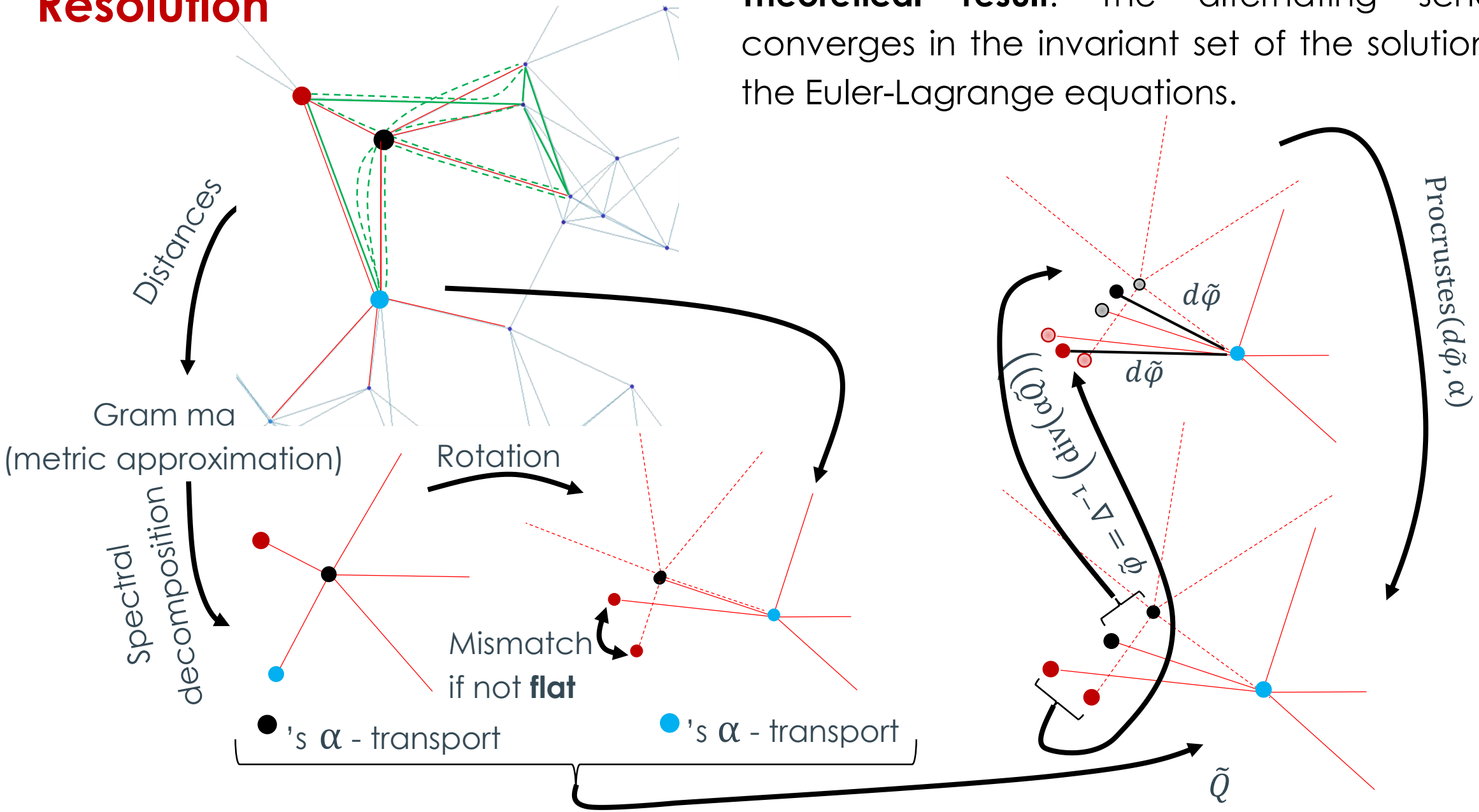
Alternating resolution

$$\varphi_{n+1} = \Delta^{-1}\mathrm{div}(\alpha Q_n)$$

$$Q_{n+1} = \mathrm{Procrustes}(d\varphi_{n+1}, \alpha)$$

Resolution

Theoretical result: The alternating scheme converges in the invariant set of the solutions of the Euler-Lagrange equations.



Implementation on distance graphs

Differential 1-forms : Linear combinations of neighborhoods' barycentric coordinates' differentials.

- **Scalar function differentials** : 1-forms with coefficients the function's differences on the graph's edges (2nd order approximation due to the barycentric constraint)
  - **Inner products of 1-forms**: The inner product of barycentric coordinates' differentials is the volume form – scaled metric pseudo-inverse.
    - **Divergence**: Inner product – dual of scalar function differential.
      - **Laplacian**: Divergence of scalar function differential

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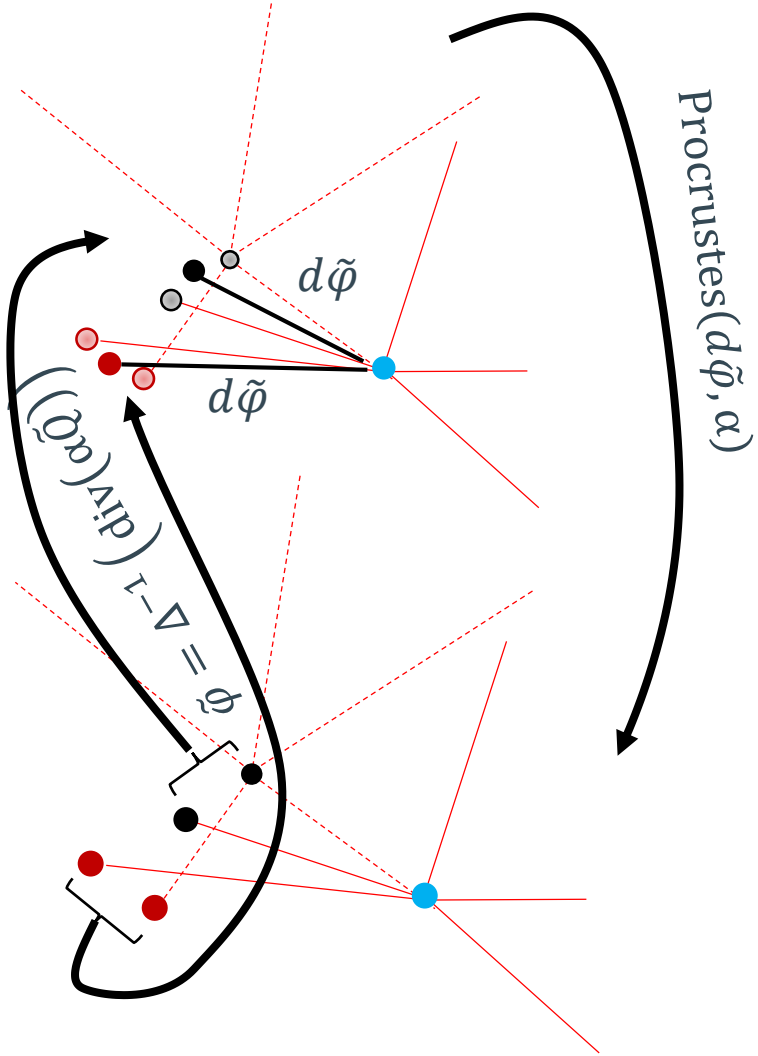
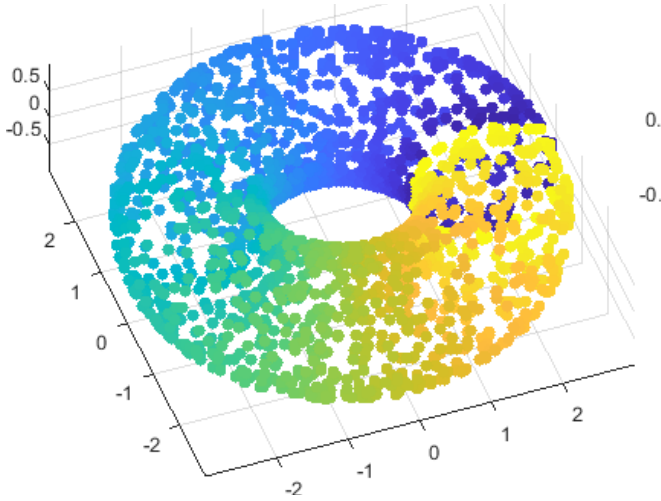
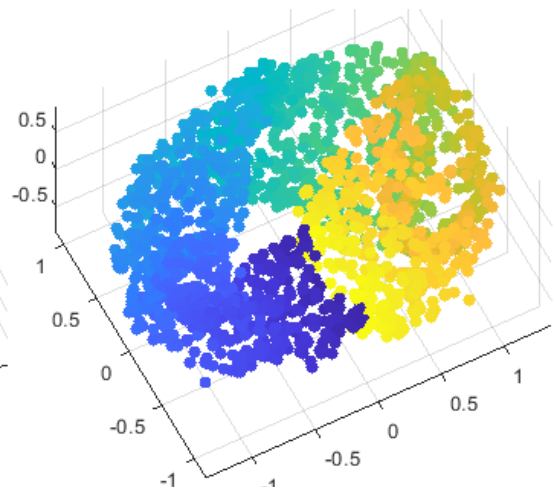


Evaluation

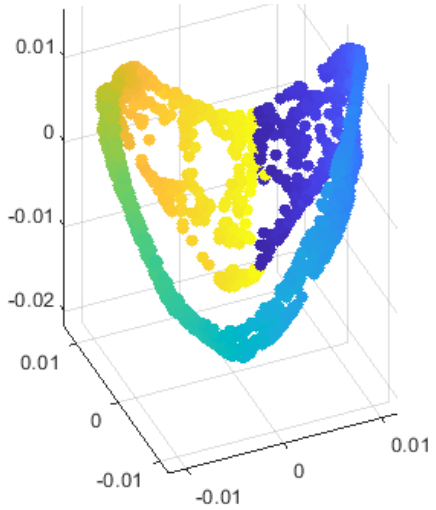
Original



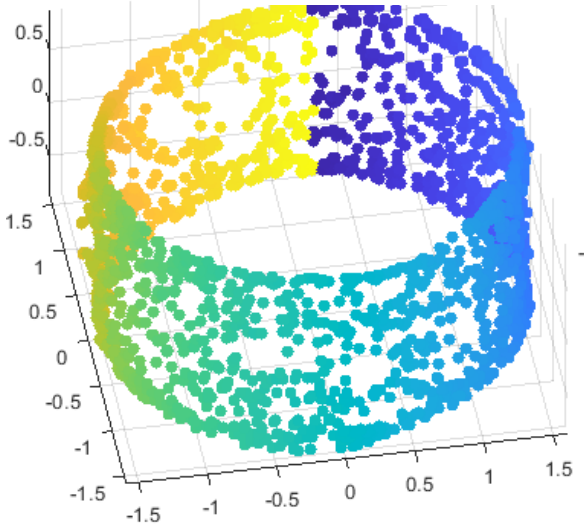
EucApprox



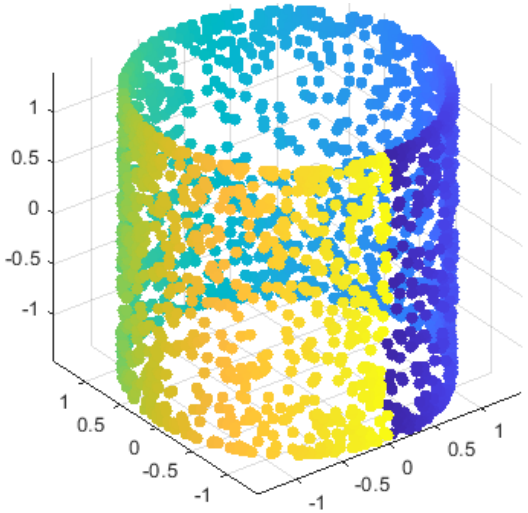
Laplacian Eigenmaps



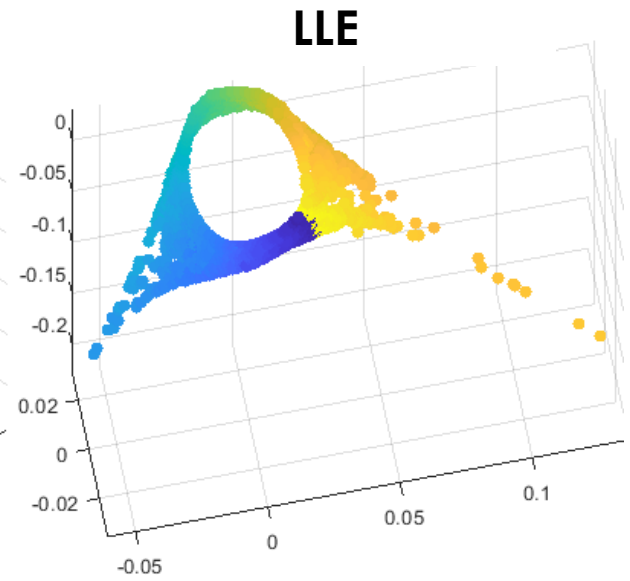
IsoMap



Diffusion Maps



LLE



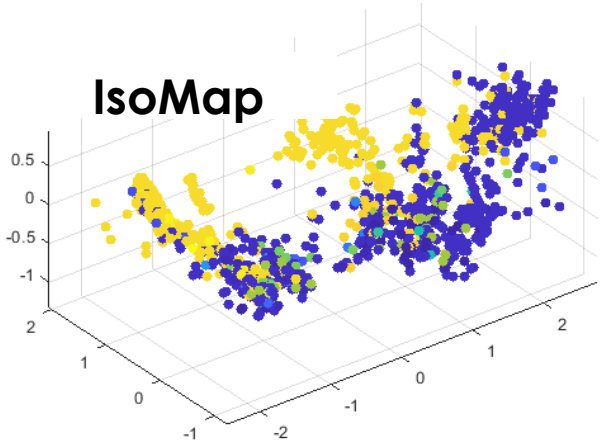
Flat torus short embedding in $\mathbb{R}^3$: Visually, EucApprox best approximates the support of the $\mathbb{R}^3$ isometry of the flat torus, while the baseline ones, either local or global, flatten one principal direction.

Evaluation

Table 2: Evaluation of the clusters' representation for the RNA-seq data set, related to lung cancer

	Diagnosis classification within embeddins' neighborhoods							
	LLE	LTSA	LplcMps	IsoMap	PHATE	t-SNE	UMAP	proposed
ACC ↑	0.6954	0.6640	0.6985	0.6825	0.6745	0.6917	0.7040	0.7126
NMI ↑	0.2934	0.2660	0.3006	0.2811	0.2952	0.3048	0.3213	0.3298
ARI ↑	0.3356	0.2525	0.3525	0.3020	0.2721	0.3461	0.3742	0.3821

IsoMap



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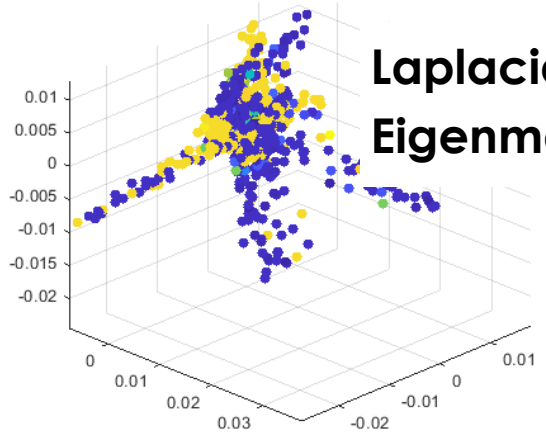
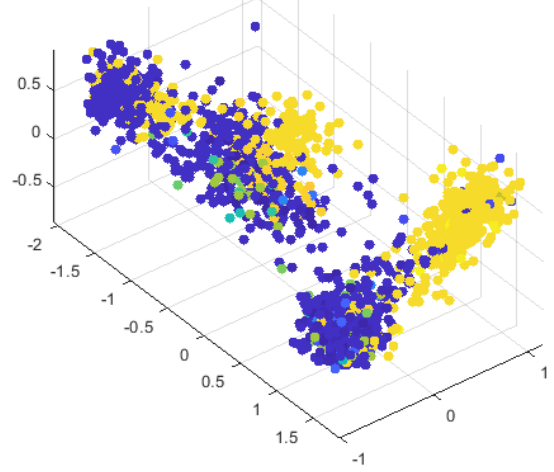
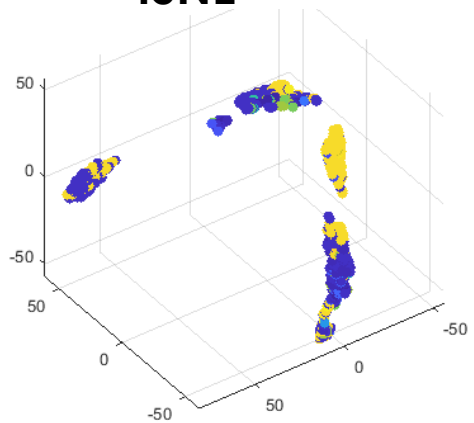


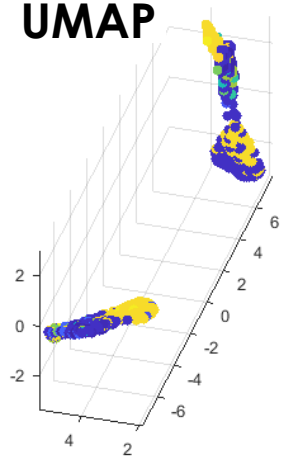
EucApprox



tSNE



UMAP



Lung cancer diagnoses' discrimination from single cell RNA data: 3D projection of the embeddings in $\mathbb{R}^{30}$. Coloring according to the lung cancer diagnosis. EucApprox respects the global distances and enhances the data discrimination by retaining local structures, up to integrability.