SpaceMAP:
Visualizing High-dimensional Data by Space Expansion

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On Machine Learning

SMACS 0723: Red arcs in the image trace light from galaxies in the very early Universe

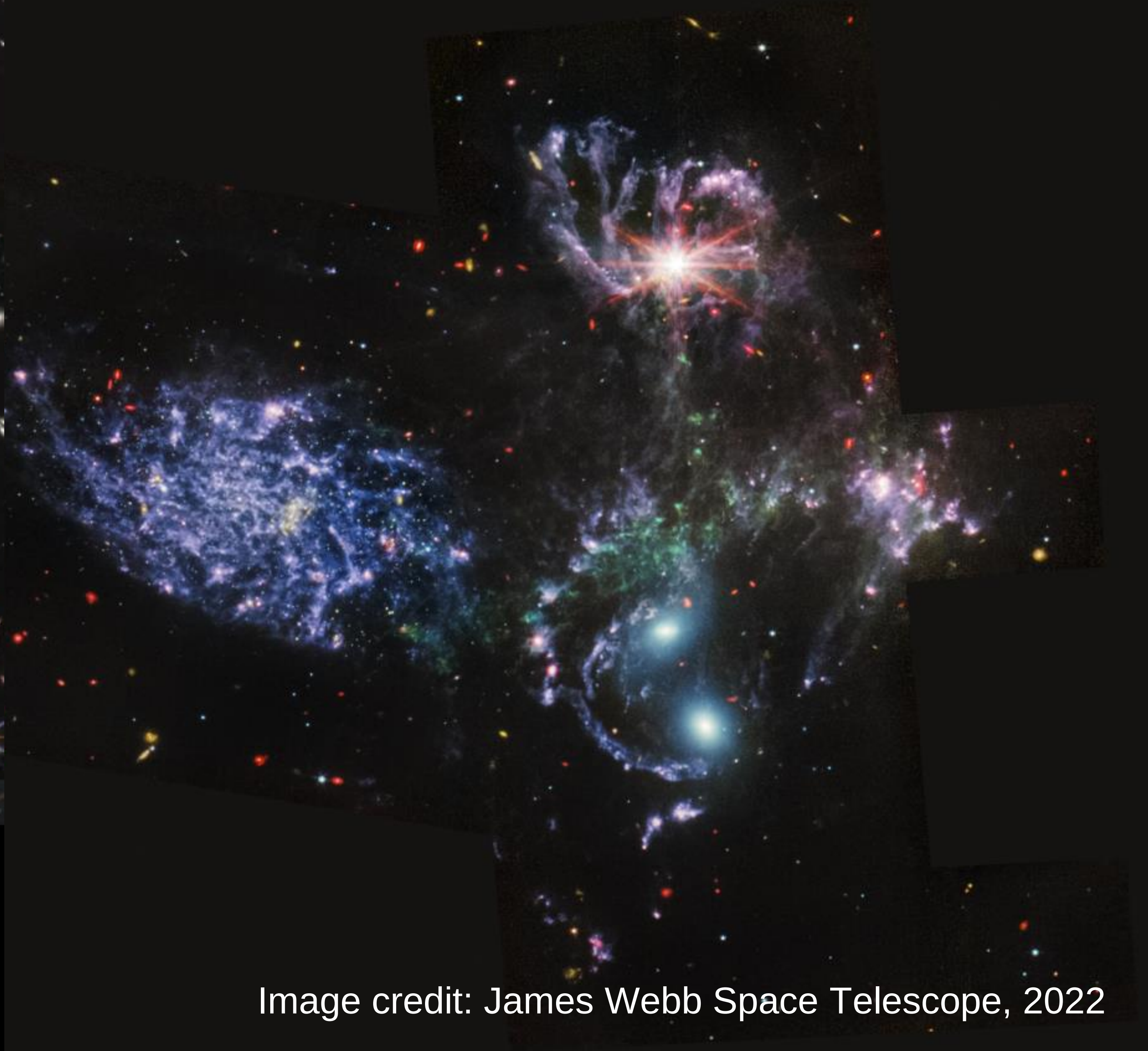


Image credit: James Webb Space Telescope, 2022

High-dimensional data visualization by SpaceMAP

What's SpaceMAP?

- SpaceMAP is a visualization / dimensionality reduction (DR) method that can see data of arbitrarily high dimension on a 2D map.

- It is based on understanding the capacity of SPACE.

- MAP refers to “manifold approximation and projection”.

Why is Visualization Interesting for ML?

- ML works based on the fundamental assumption that data lies on a low-dimensional manifold – otherwise “curse of dimensionality” holds

- Seeing is believing – as human we only can “see” well in 2 or 3 dimension, hence data visualization is super interesting for ML’ers!

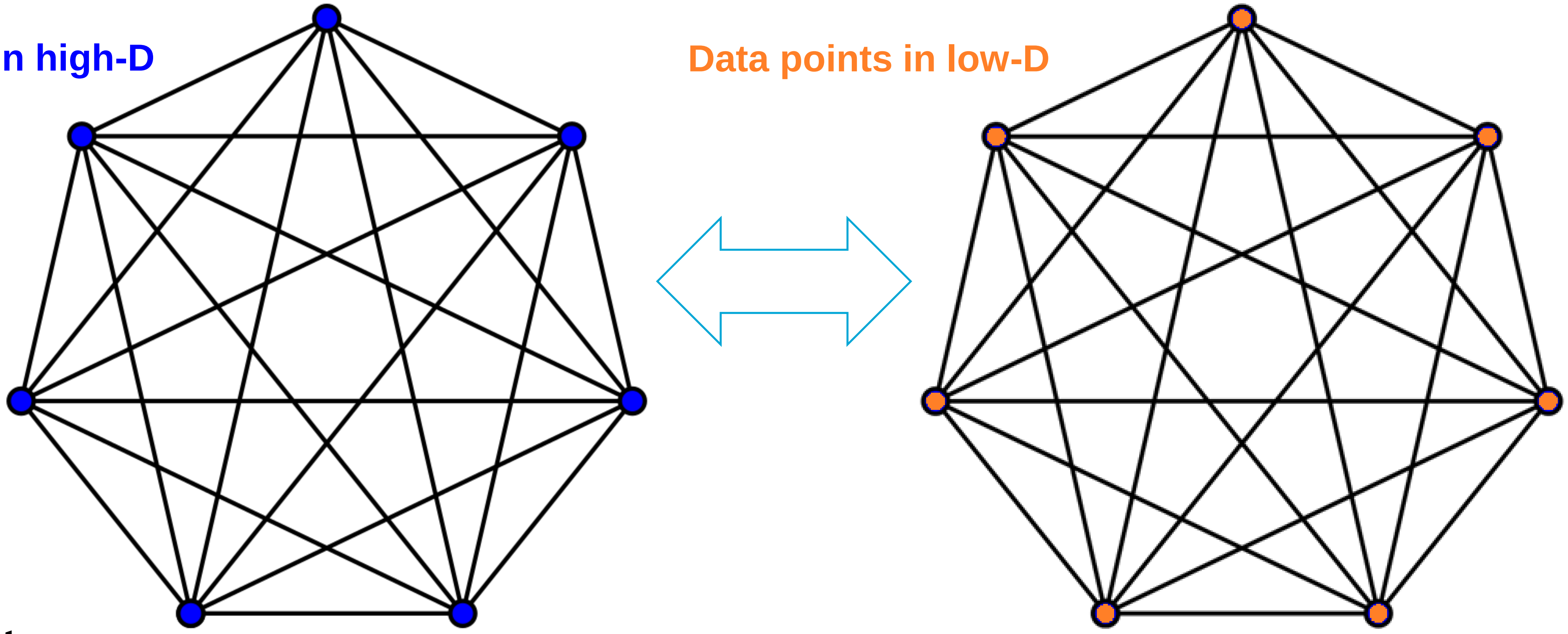
What's New in SpaceMAP?

- The discrepancy between high-D and low-D spaces is analytically studied, leading to transformation of similarity in a principled and explainable way.

- In contrast, previous methods such as t-SNE and UMAP transformed similarity implicitly.

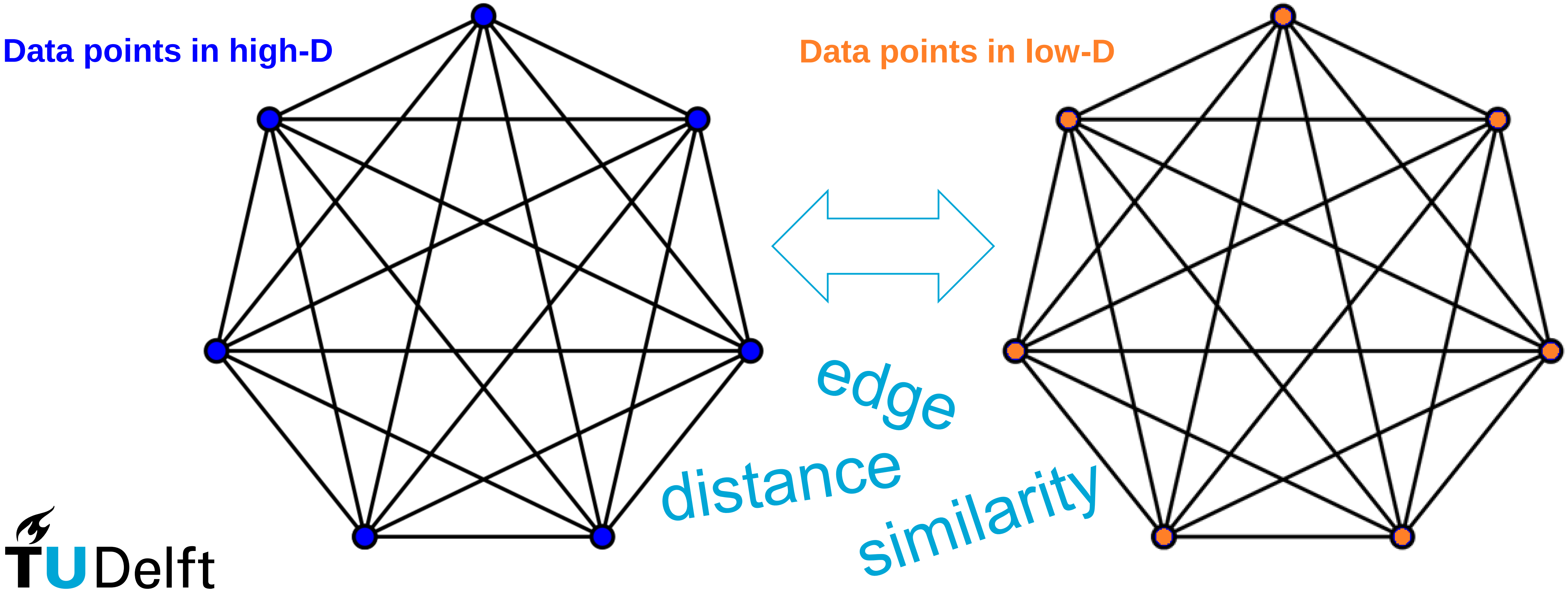
The Essence of Dimensionality Reduction

- Matching two graphs



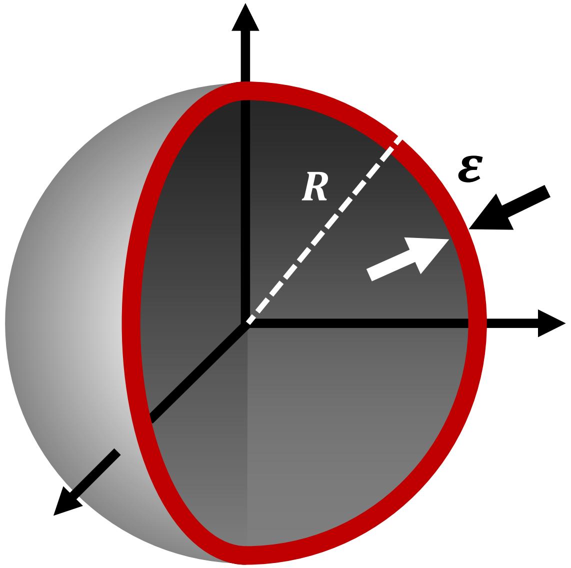
The Essence of Dimensionality Reduction

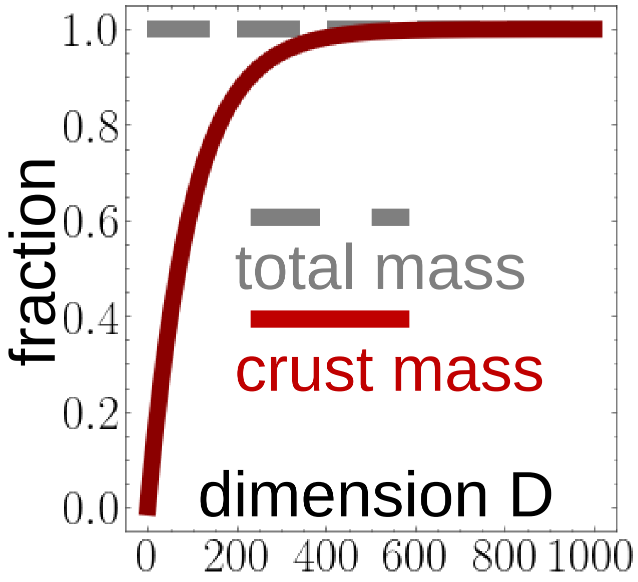
- Matching two graphs



The Crowding Problem of Dimensionality Reduction

- **high-dimensional** geometry: **“concentration on a crust”**



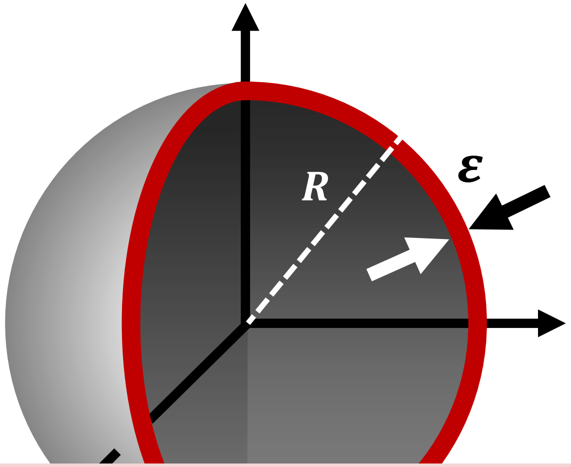


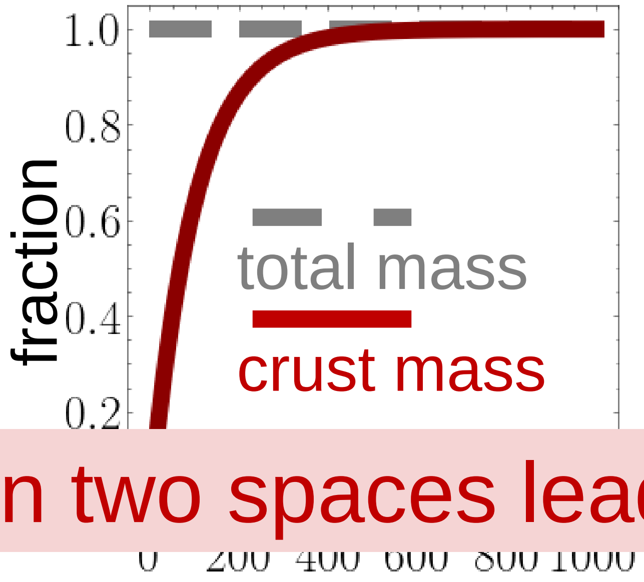
causes

- General difficulty in DR: **the “crowding problem”**

The Crowding Problem of Dimensionality Reduction

- **high-dimensional** geometry: **"concentration on a crust"**





Distance defined the same way in two spaces lead to problems!

causes

- General difficulty in DR: **the "crowding problem"**

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SpaceMAP: the Theoretic Framework

- Space Capacity $\boldsymbol{\mathcal{V}_D(R_{ij})}$
  - A Hausdorff measure - volume of a D-dim ball
- Equivalent Extended Distance (EED) $\tilde{\mathcal{R}}_{ij,D\to d}$
  - Transform the distance in low-D space such that capacity matches to low-D space: $\mathcal{V}_d(\tilde{\mathcal{R}}_{ij,D\to d}) = \mathcal{V}_D(R_{ij})$

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SpaceMAP: the Theoretic Framework

- Space Capacity $\mathcal{V}_D(R_{ij})$
  - A Hausdorff measure - volume of a D-dim ball

Definition 3.1 (Space Capacity). *Let $R_{ij} = l(\boldsymbol{x}_i, \boldsymbol{x}_j) \in \mathbb{R}$ be the distance between data point $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ in the D-dimensional space. The space capacity $\mathcal{V}_D(R_{ij})$ from point i to point j is defined as the volume of a D-dimensional ball with a radius of R_{ij}.*

- Equivalent Extended Distance
  - Transform the distance in low-D space such that capacity matches to low-D space: $\mathcal{V}_d(\tilde{\mathcal{R}}_{ij,D\to d}) = \mathcal{V}_D(R_{ij})$

$$\tilde{\mathcal{R}}_{D\to d} = \alpha R^{\frac{D}{d}}$$

Definition 3.2 (Equivalent Extended Distance: EED). *Let $R_{ij} = l(\boldsymbol{x}_i, \boldsymbol{x}_j) \in \mathbb{R}$ be the distance between data point $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ in the D-dimensional space. The equivalent extended distance (EED) $\tilde{\mathcal{R}}_{ij,D\to d}$ is defined as the equivalent distance between $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ in d-dimensional space such that the Space Capacity matches: $\mathcal{V}_d(\tilde{\mathcal{R}}_{ij,D\to d}) = \mathcal{V}_D(R_{ij})$*

SpaceMAP: the Theoretic Framework

- Intrinsic Dimension (ID)
  - Inherent degrees of freedom of data

- EED provably transforms ID
  - By applying EED $\mathcal{V}_d(\tilde{\mathcal{R}}_{ij,D\to d}) = \mathcal{V}_D(R_{ij})$, the ID of data is transformed to be visualizable with mitigated “crowding problem”

SpaceMAP: the Theoretic Framework

- Intrinsic Dimension (ID) Estimation
  - Inherent degrees of freedom of data

$$\hat{d}_k(x_i; R) = \left(\frac{1}{k-1} \sum_{j=1}^{k-1} \log \frac{R_{ik}}{R_{ij}} \right)^{-1}$$

Levina & Bickel 2004

- EED provably transforms ID
  - By applying EED $\mathcal{V}_d(\tilde{\mathcal{R}}_{ij,D\to d}) = \mathcal{V}_D(R_{ij})$, the ID of data is transformed to be visualizable with mitigated “crowding problem”

Proposition 3.1 (EED transforms ID provably). *For any neighborhood size k, if the MLE of the intrinsic dimension around point x_i under the distance metric R is $\hat{d}_k(x_i; R) = D$, the MLE of the intrinsic dimension after applying EED to the distance metric is d: $\hat{d}_k(x_i; \tilde{\mathcal{R}}_{D\to d}) = d$.*

Proof. By replacing metric R with the EED-transformed metric $\tilde{\mathcal{R}}_{D\to d}$ (Equation 4) in Equation 5, we have:

$$\begin{aligned}\hat{d}_k(x_i; \tilde{\mathcal{R}}_{D\to d}) &= \left(\frac{1}{k-1} \sum_{j=1}^{k-1} \log \frac{\alpha R_{ik}^{D/d}}{\alpha R_{ij}^{D/d}} \right)^{-1} \\ &= \left(\frac{1}{k-1} \sum_{j=1}^{k-1} \frac{D}{d} \log \frac{R_{ik}}{R_{ij}} \right)^{-1} \\ &= \frac{d}{D} \hat{d}_k(x_i; R) = \frac{d}{D} D = d \qquad (7)\end{aligned}$$

□

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SpaceMAP: the Method

■ Definitions in SpaceMAP:

Space Capacity

$\mathcal{V}_D(R_{ij})$ Volume of a D-dim ball

↓

Equivalent Extended Distance (EED)

$\tilde{\mathcal{R}}_{D\to d}$ s.t. $\mathcal{V}_D(R_{ij}) = \mathcal{V}_d(\mathcal{R}_{D\to d})$

Estimation of ID

$\hat{\mathbf{d}}_{\mathbf{k}}$ k: number of neighbors

↓

Local/Global ID

$d_{local}(x_i; k) = \hat{d}_k$

d_{global} Harmonic mean of d_{local}

■ Algorithm:

① Calculate local/global **ID** → ② Use **ID** to obtain **EED** among the data points → ③ Shape the similarity functions (**P**/**Q**) to achieve **EED** using **local/global ID**

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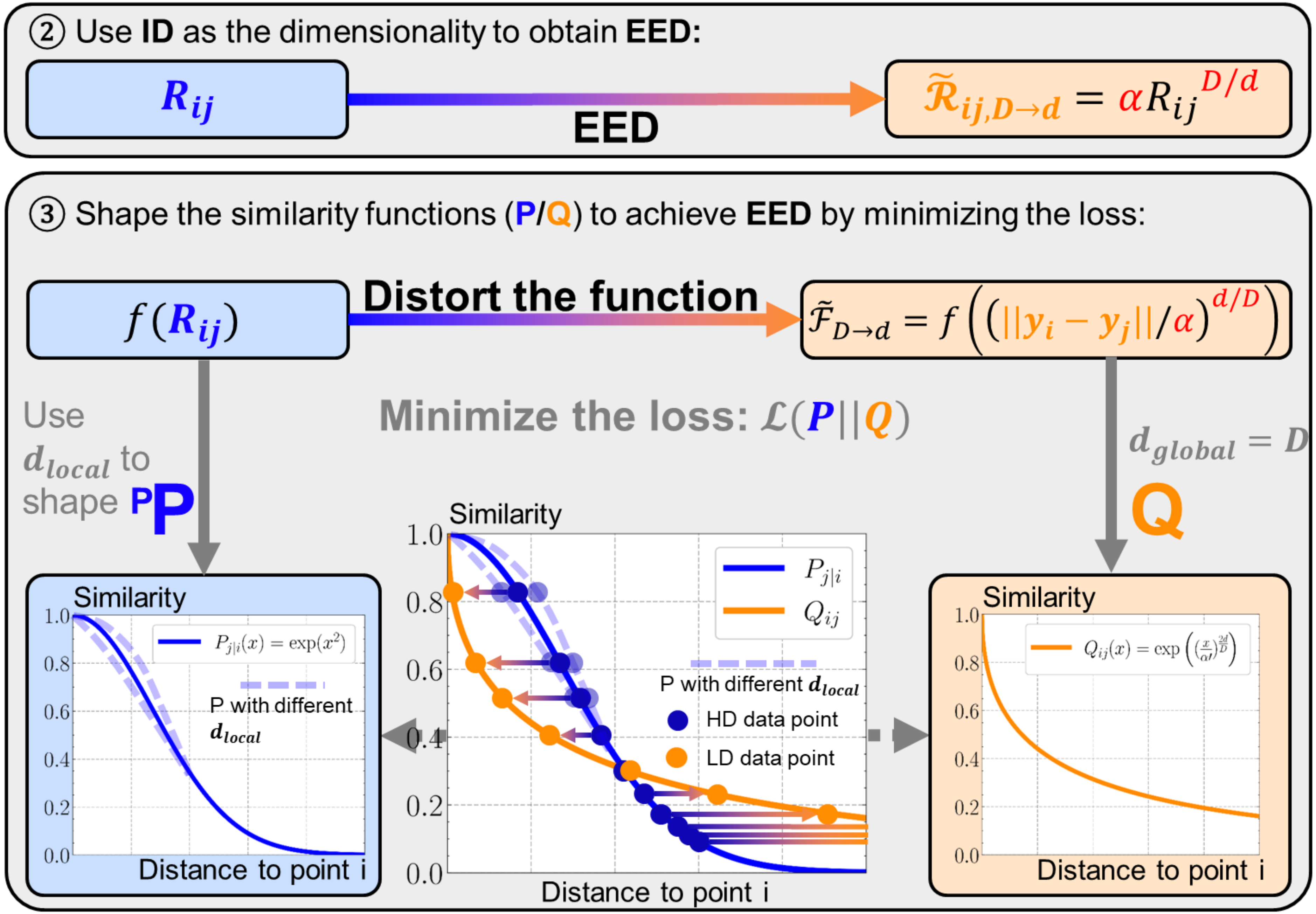
SpaceMAP: the Method



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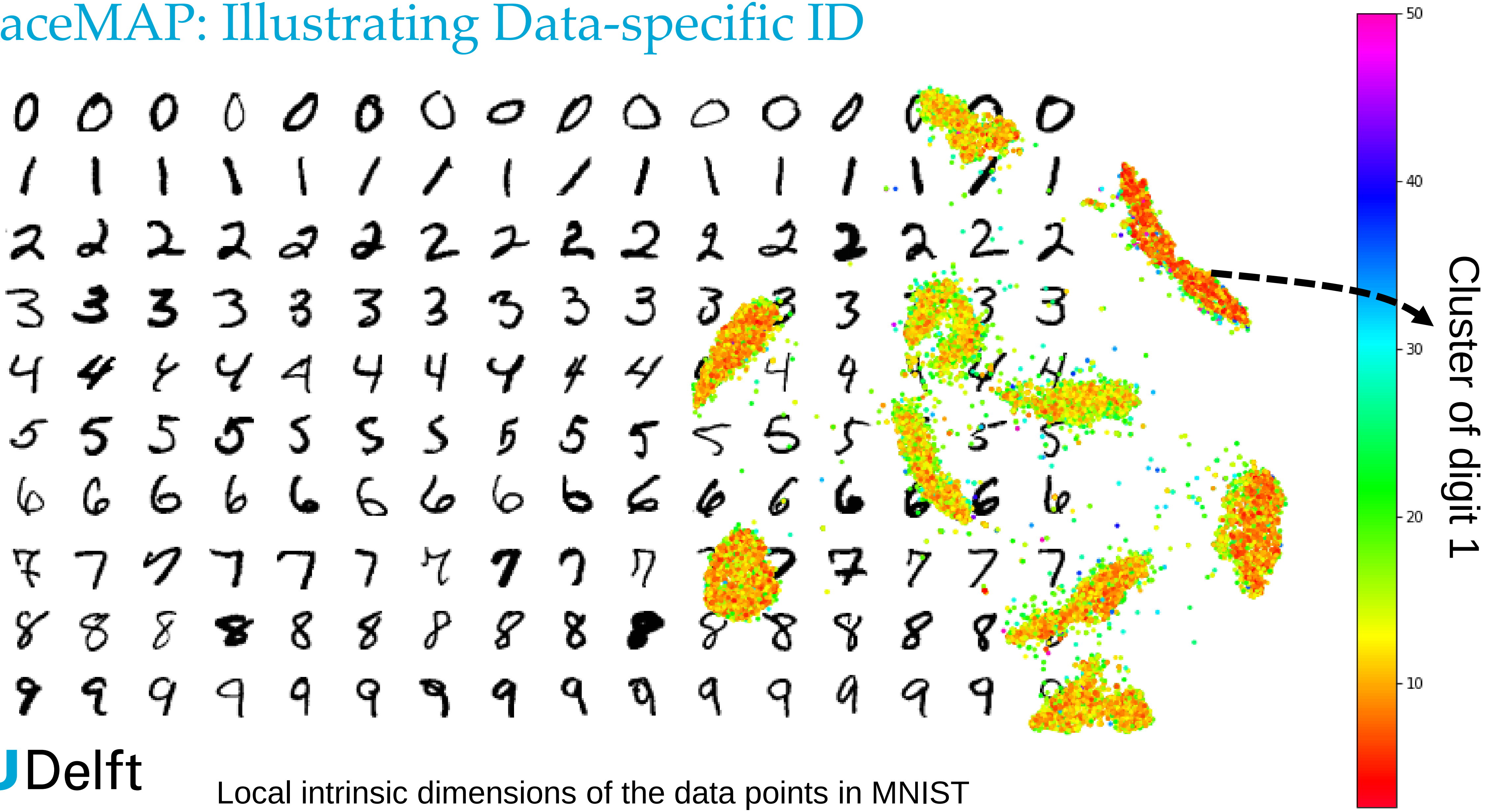
SpaceMAP: Illustrating Data-specific ID



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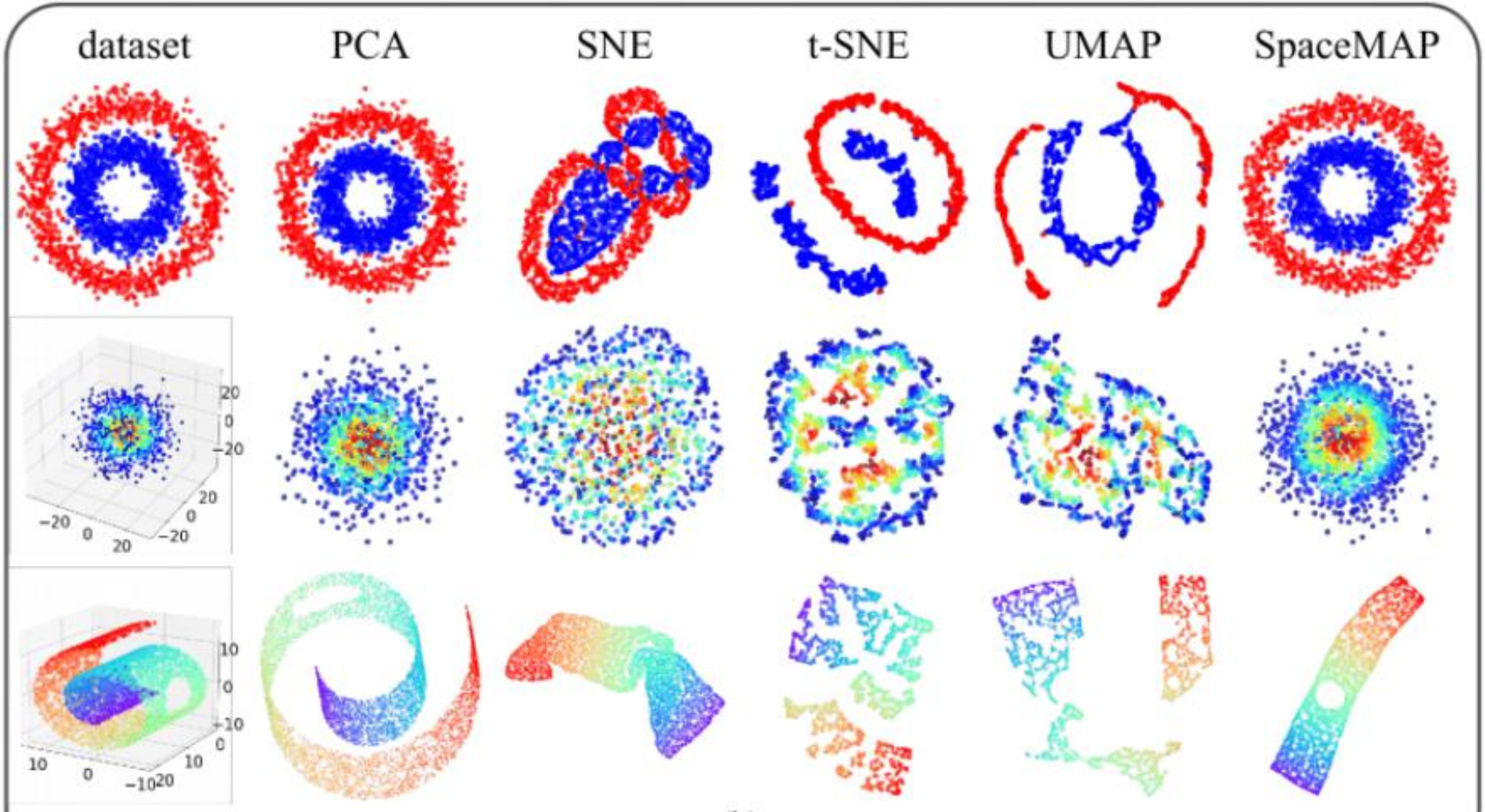
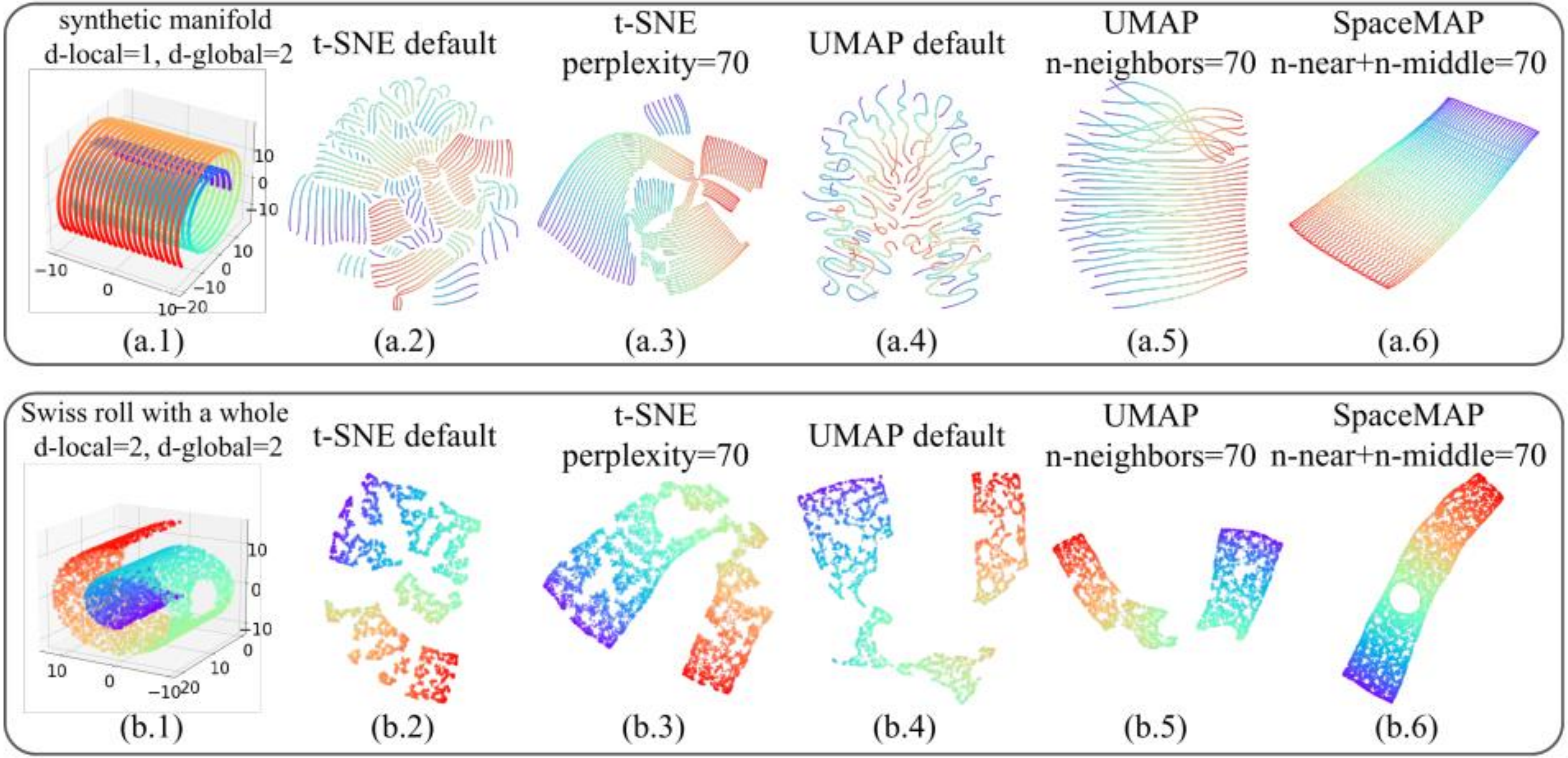
Local intrinsic dimensions of the data points in MNIST

SpaceMAP Results

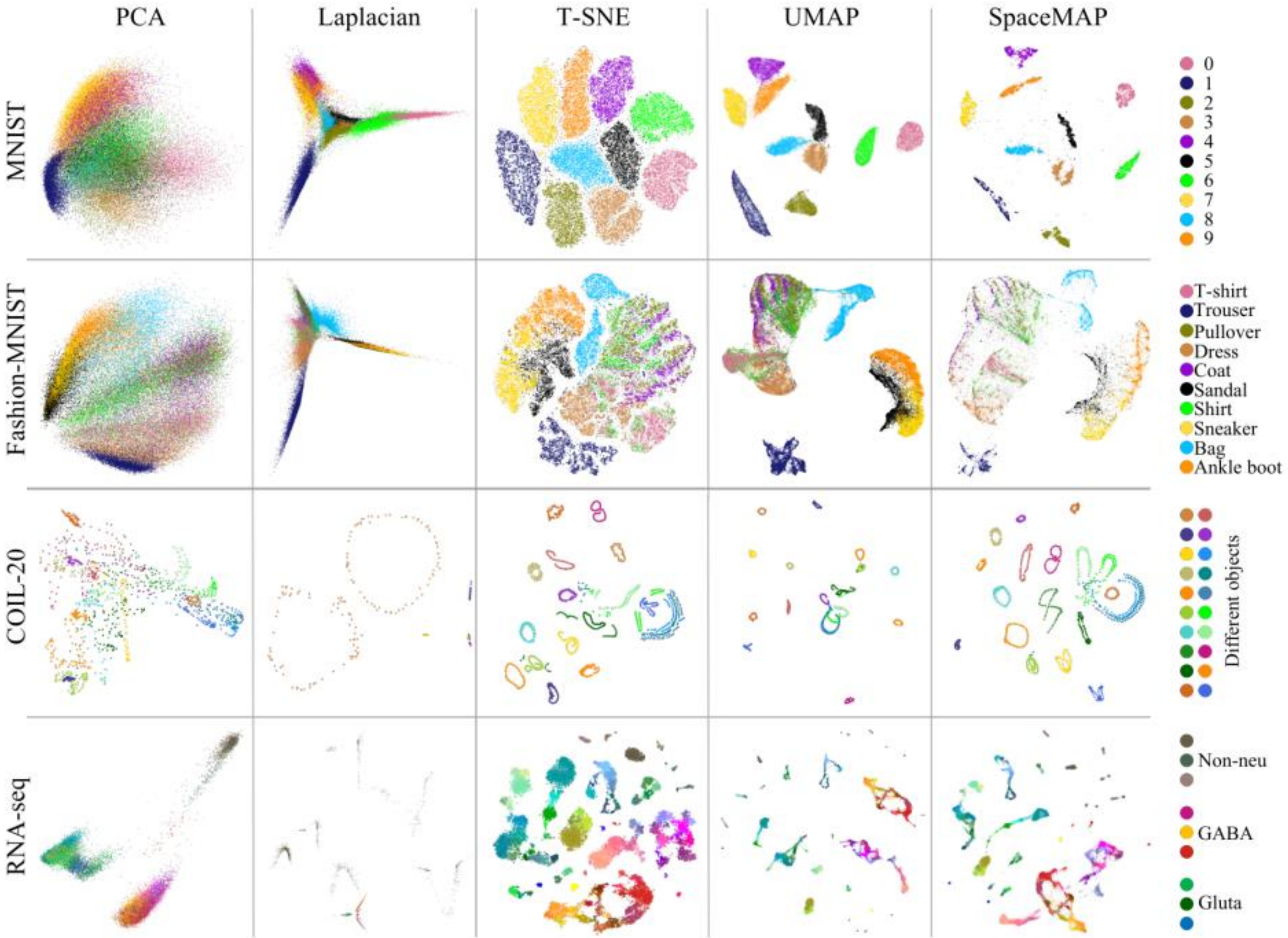


(b)

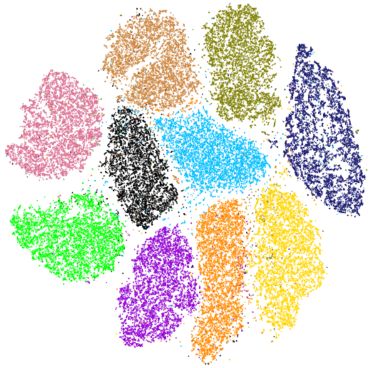
SpaceMAP Results



SpaceMAP


PCA
Laplacian
T-SNE
UMAP
SpaceMAP
MNIST
Fashion-MNIST
COIL-20
RNA-seq
0
1
2
3
4
5
6
7
8
9
T-shirt
Trouser
Pullover
Dress
Coat
Sandal
Shirt
Sneaker
Bag
Ankle boot
Different objects
Non-neu
GABA
Gluta

SpaceMAP Results



t-SNE result

UMAP result

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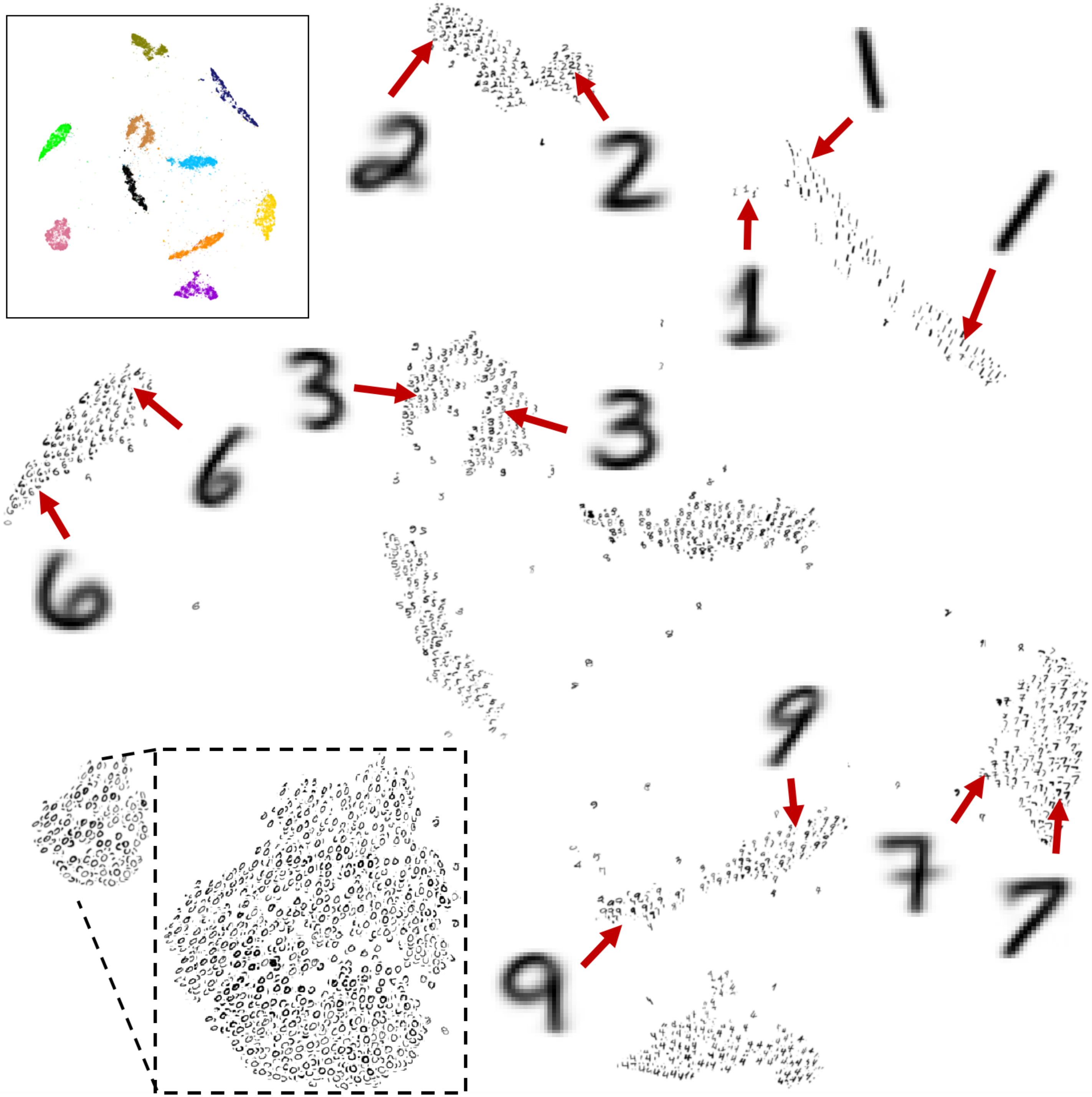
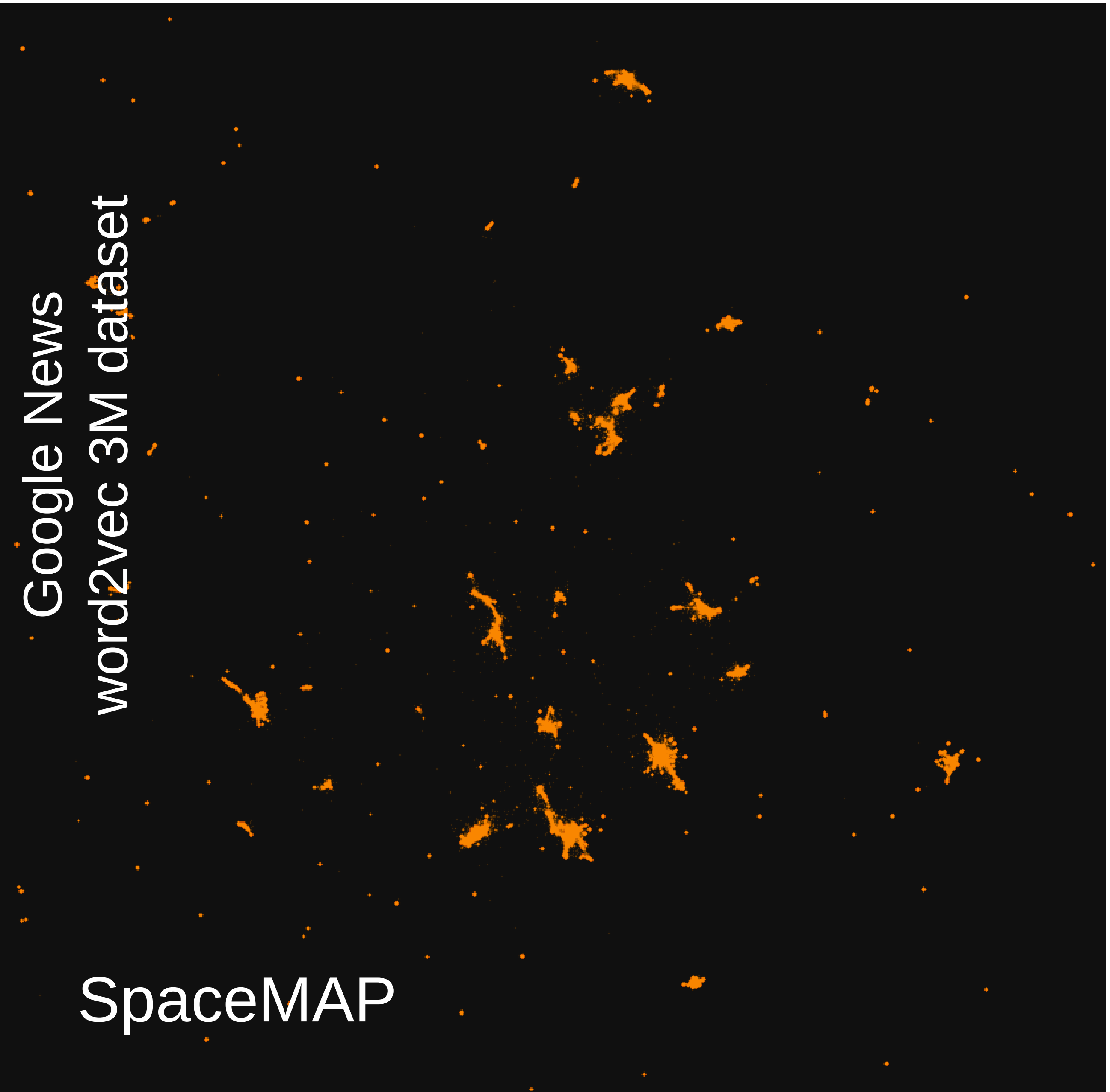
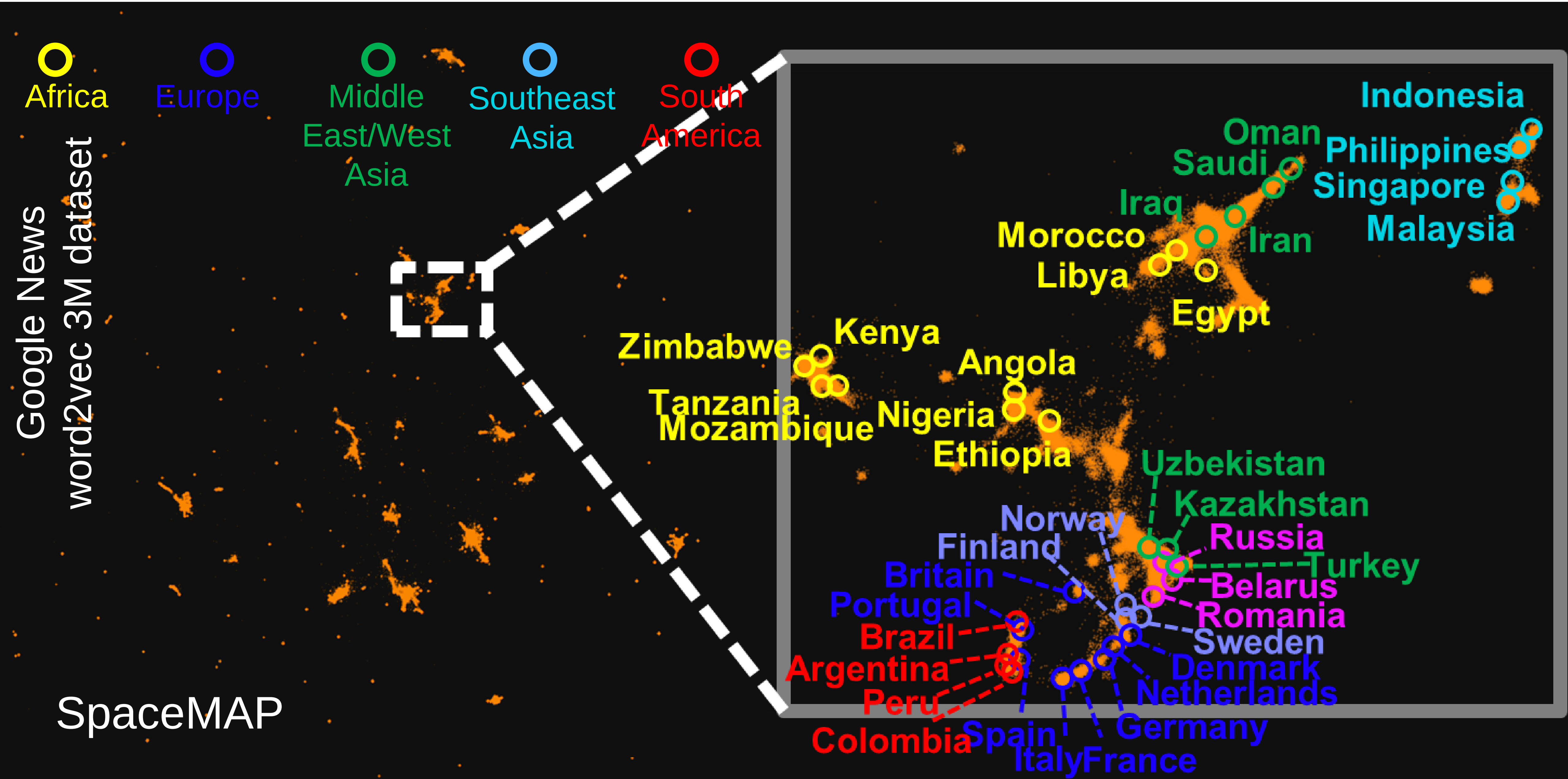


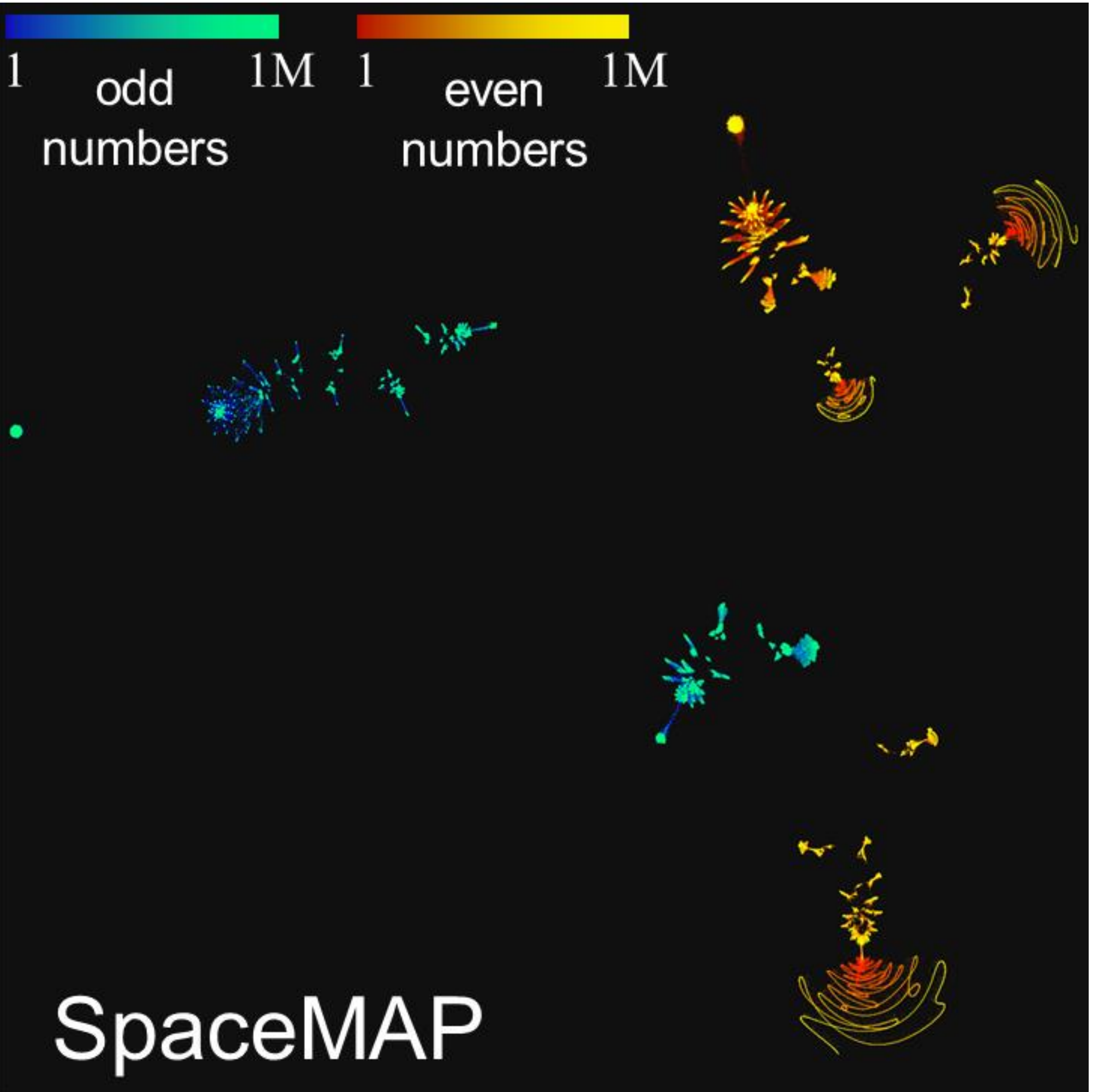
SpaceMAP Results: the Word Map



SpaceMAP Results: the Word Map – World Map



SpaceMAP Results



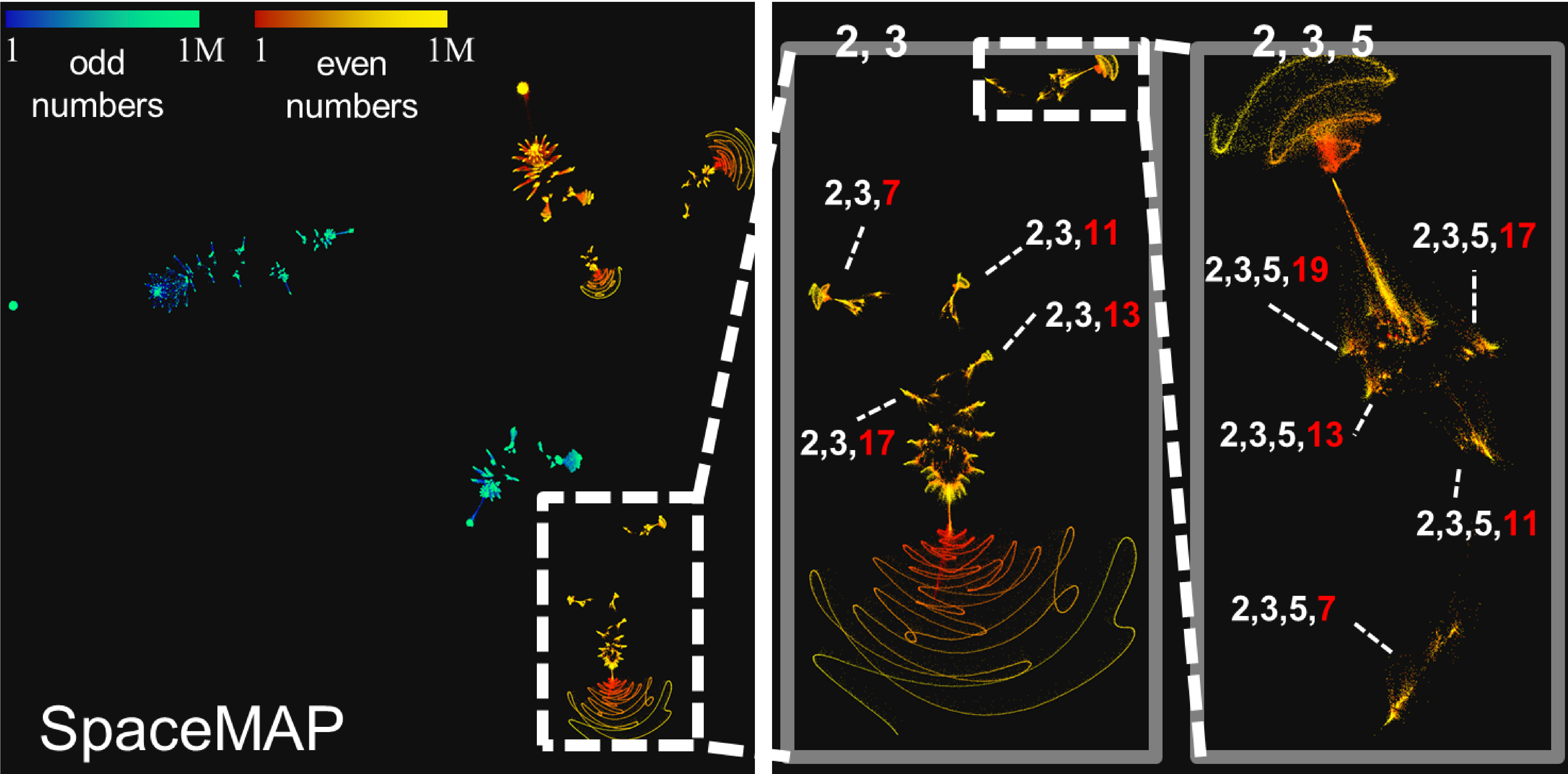
Divisibility by prime numbers:

- A binary vector showing the divisibility of positive integer from 1 to 1,000,000 by prime number 2, 3, 5,…, 999983

UMAP McInnes et al. 2018

- 78498-dimensional binary vector
- Visualized in 2D SpaceMAP

SpaceMAP Results



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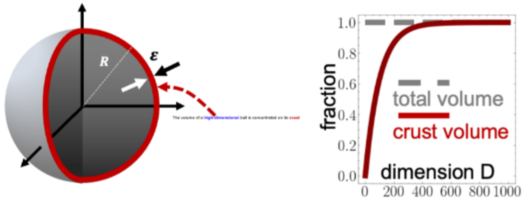
Poster #623

Dimensionality Reduction (DR) and Intrinsic Dimension (ID)

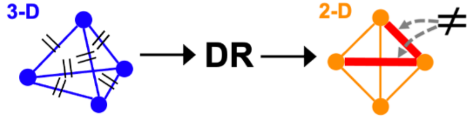
- Dimensionality Reduction (**DR**) translates **high-dimensional data** into **low-dimensional space** <2-D/3-D for visualization>.
- Intrinsic dimension (**ID**) is the internal degrees of freedom of data <usually larger than 3-D>.

'Concentration on a Crust' and the 'Crowding Problem'

- **high-dimensional** geometry: **'concentration on a crust'**:



- General difficulty in DR: **the 'crowding problem'**:



The distances between high-dimensional data points are **concentrated**, which are **difficult to preserve** in low-dimensional spaces.

Our Main Contribution

- **Analytically** alleviate the crowding problem in a data-specific manner.
- Hierarchical manifold approximation by estimating **local/global ID**.

Proposition (EED transforms ID provably)

- For any dataset with $ID = D$, if we apply EED $\tilde{\mathcal{R}}_{D\to d}$, then $ID = d$.

High-dimensional dataset with distances: R_{ij} — ID: D → EED → Dataset with EED distances: $\tilde{\mathcal{R}}_{ij,D\to d} = \alpha R_{ij}^{D/d}$ — ID: d

√ **The extended distances are easier to embed in the d-dimensional space!**

Methodology

- Definations in SpaceMAP:

Space Capacity $\mathcal{V}_D(R_{ij})$ Volume of a D-dim ball

Equivalent Extended Distance (EED) $\tilde{\mathcal{R}}_{D\to d}$ s.t. $\mathcal{V}_D(R_{ij}) = \mathcal{V}_d(\mathcal{R}_{D\to d})$

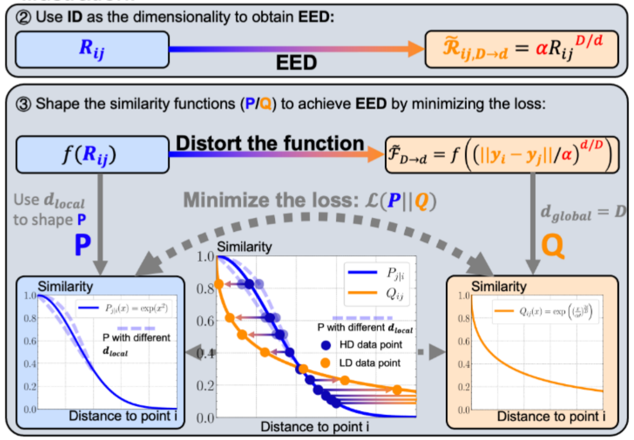
Estimation of ID $\hat{d}_k$ k: number of neighbors

Local/Global ID $d_{local}(x_i; k) = \hat{d}_k$; d_{global} Harmonic mean of d_{local}

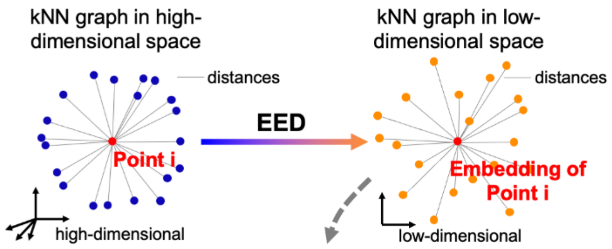
- Algorithm:

① Calculate local/global ID → ② Use ID to obtain EED among the data points → ③ Shape the similarity functions (P/Q) to achieve EED using local/global ID

- Illustration:

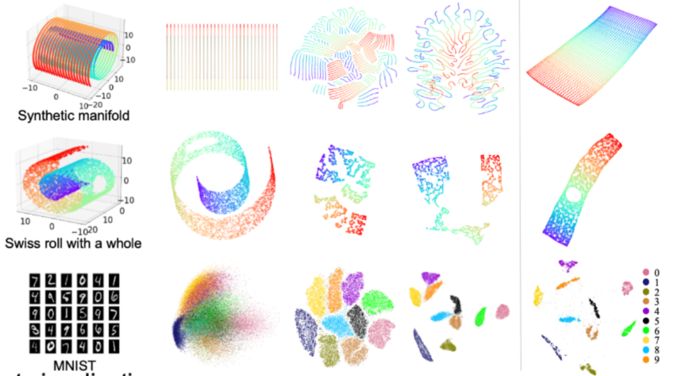


A Simple Example

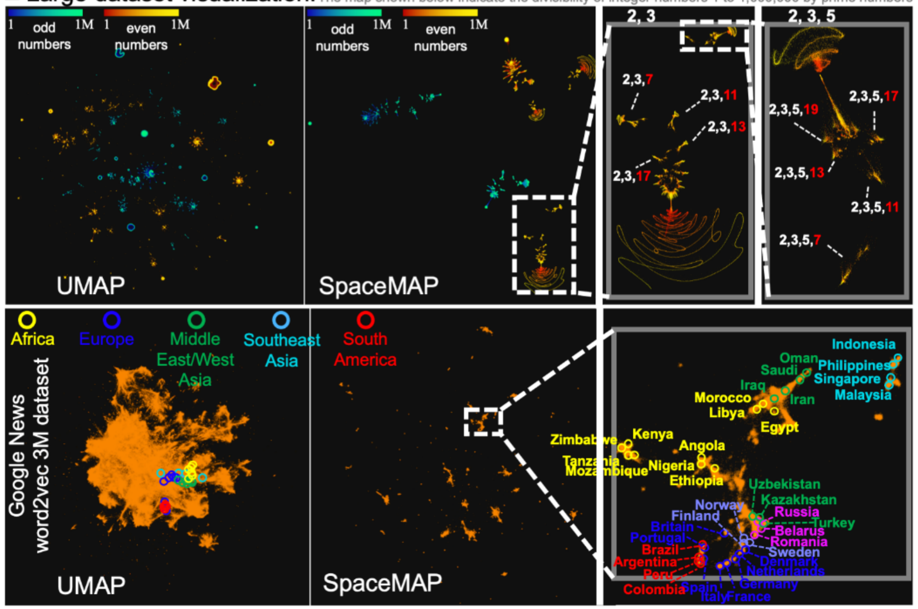


Results

- Visualization results:



- Large dataset visualization: The map shown below indicate the divisibility of integer numbers 1 to 1,000,000 by prime numbers



Conclusion

- We introduce the definitions of **space capacity**, **intrinsic dimension (ID)** and **equivelant extended distance (EED)** and utilize them to transform distances between high- and low-dimensional spaces and alleviate the 'crowding problem' analytically.
- We model the hierarchical structure in a dataset-specific manner based on the **local and global IDs** of data.

S P A C E M A P

- Space Capacity
- Intrinsic Dimension (ID)
- Equivalent Extended Distance (EED)
- Data-specific Manifold