Reduction of dimension

PCA, LLE, tSNE, UMAP

Copernicus master

2025–2026

Thomas Corpetti

Outline

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Principal Component Analysis

- **Problem** : In statistical learning, we accumulate P measurements of N variables (color, contrast, ...). We obtain a data matrix X of size $P \times N$.

  $\Longrightarrow$ How to **visualize** this data when $N > 2$?

  $\Longrightarrow$ How to retain only the **useful** information ?

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- **Principle of PCA** : Represent the information along the axes with the highest variance.

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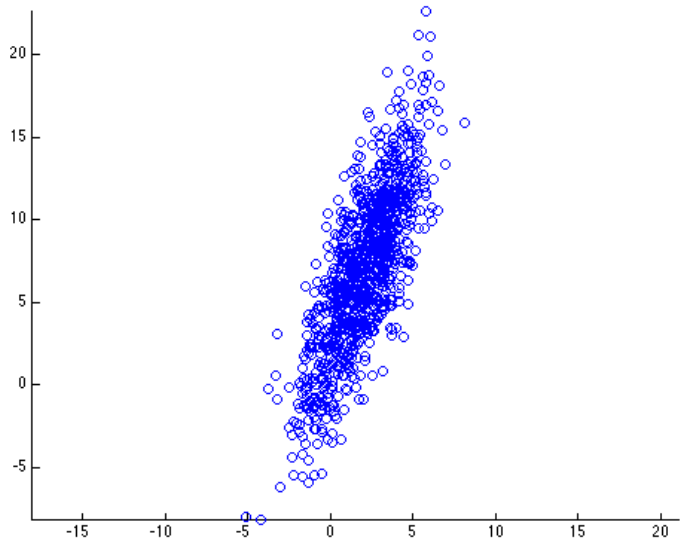

Principal Component Analysis : How Does It Work ?

- **Objective** : Find the axes that explain the maximum variance of all the data. Input data :

$$X = \begin{bmatrix} X_{1,1} & ... & X_{1,N} \\ ... & ... & ... \\ X_{P,1} & ... & X_{P,N} \end{bmatrix}$$

- **Center of Mass** of matrix X :

$$g = [\overline{X_1}, ..., \overline{X_N}]^T$$

- **Centered Matrix** (with $\mathbf{1} = [1, 1, ..., 1]^T$) :

$$\overline{X} = \begin{bmatrix} X_{1,1} - \overline{X_1} & ... & X_{1,N} - \overline{X_N} \\ ... & ... & ... \\ X_{P,1} - \overline{X_1} & ... & X_{P,N} - \overline{X_N} \end{bmatrix} = X - \mathbf{1}g^T$$

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Principal Component Analysis : How Does It Work ?

- **Standardized Centered Matrix** :

$$\widetilde{X} = \begin{bmatrix} \frac{X_{1,1}-\overline{X_1}}{\sigma(X_1)} & \cdots & \frac{X_{1,N}-\overline{X_N}}{\sigma(X_1)} \\ \cdots & \cdots & \cdots \\ \frac{X_{P,1}-\overline{X_1}}{\sigma(X_1)} & \cdots & \frac{X_{P,N}-\overline{X_N}}{\sigma(X_N)} \end{bmatrix}$$

- To Standardize or Not to Standardize the Matrix ?
  - If not : a variable with high variance will dominate everything.
  - If yes : we may give importance to noisy data.

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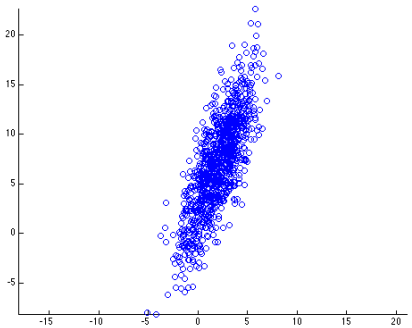

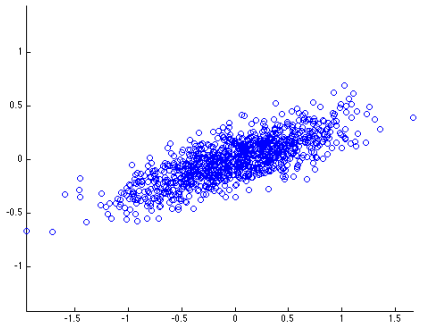

Not Standardized Standardized Centered

Principal Component Analysis : How Does It Work ?

- **Matrix of Correlations or Covariances** M (with $K = P - 1$) :

$$M = \frac{1}{K} W^T W$$

- Matrix is **square, symmetric, and real**.
- Let Λ be the diagonal matrix of eigenvalues of M arranged in descending order, and Q the matrix of associated eigenvectors.
- The **vector that explains the most inertia** in the cloud is the first eigenvector (same for the others).
- The variance explained by the k-th eigenvector is λ_k.

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Principal Component Analysis : Key Takeaways

We have a cloud of points (centered/reduced, as needed) represented by W.

- The **Matrix of Correlations or Covariances** M is defined as (with $K = P - 1$) :

$$M = \frac{1}{K} W^T W$$

- The orthonormal basis Q that explains the most variance is represented by the matrix of **unit eigenvectors associated with eigenvalues, arranged in descending order**.
- The variance explained by each component corresponds to its associated eigenvalue.
- Coordinates of W in the new basis : $W' = Q^T W$

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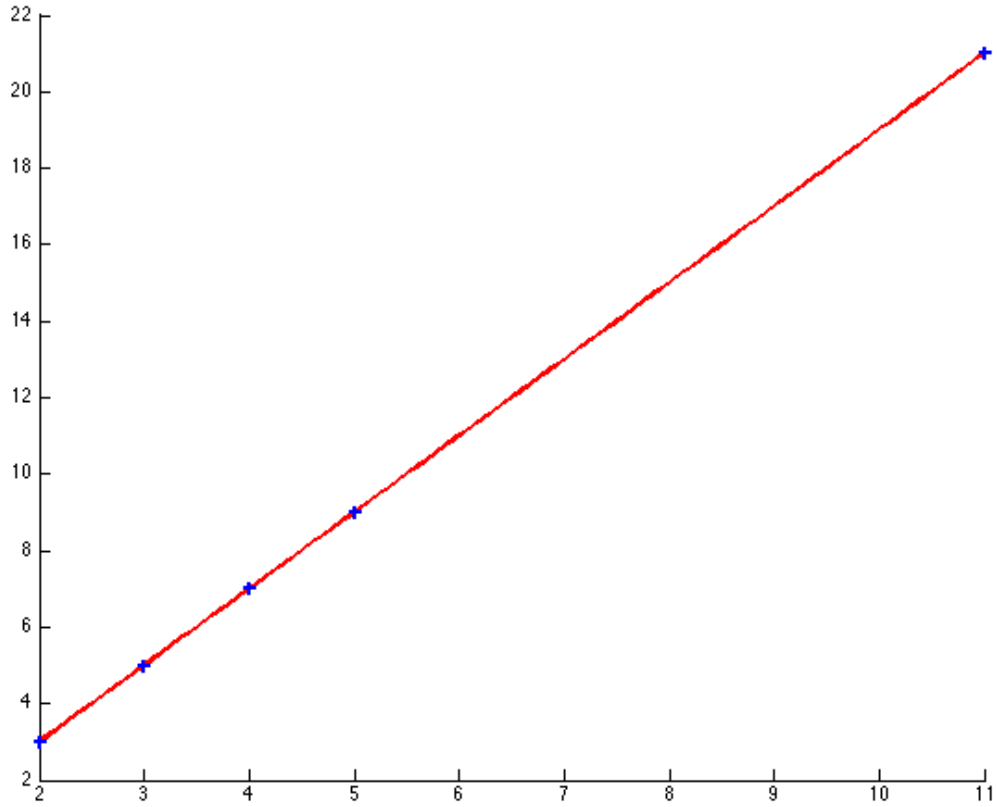
Principal Component Analysis : Exercises

We have the following dataset of points :

$$X = \begin{bmatrix} 2 & 3 \\ 5 & 9 \\ 4 & 7 \\ 3 & 5 \\ 11 & 21 \end{bmatrix}$$

1. What are the principal axes (we decide to center but not reduce) ?
2. What are the coordinates of these points in the basis composed of the principal components ?
3. What is the coefficient of correlation ?
4. What conclusions can we draw ?



Dispersion of the data along a perfect straight line

Principal Component Analysis : Exercises

We have the following data points :

$$X = \begin{bmatrix} 1 & 1 \\ 2 & 5 \\ 4 & 7 \\ 5 & 11 \end{bmatrix}$$

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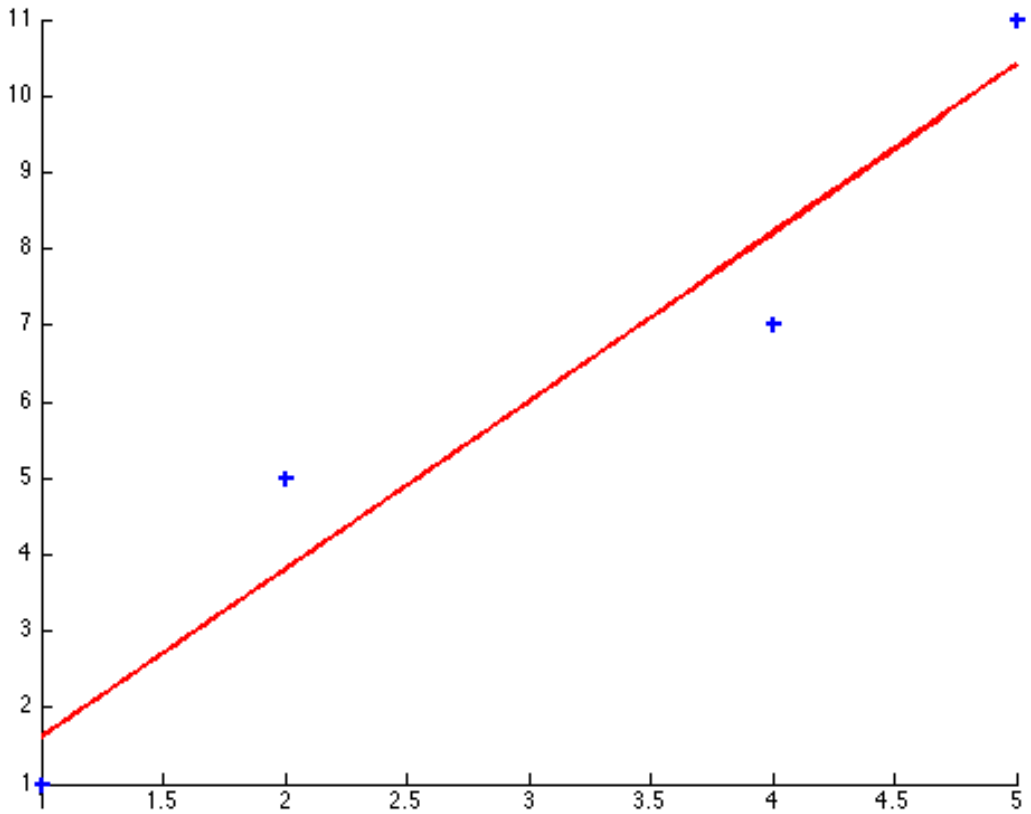

Dispersion of points

Principal Component Analysis : Exercises

Course Grades : We consider the following table of course grades

	Maths	Physics	French	Languages	Music
Erwan	6	6	5	5.5	8
Armelle	8	8	8	8	9
Rudy	6	7	11	9.5	11
Albert	14.5	14.5	15.5	15	8
Didier	14	14	12	12	10
Nicolas	11	10	5.5	7	13
Hélène	5.5	7	14	11.5	10
Catherine	13	12.5	8.5	9.5	12
Ronan	9	9.5	12.5	12	18

Averages

Maths	Physics	French	Languages	Music
9.67	9.83	10.22	10.00	11.00

See `https://tinyurl.com/47cvvauw`

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Principal Component Analysis : Exercises

We want to perform PCA on the grade table.

Here is the covariance matrix

```
mat_var_cov =

   12.8125   11.1562    2.9896    5.1562    0.1250
   11.1562   10.0625    4.6354    5.9062    0.0625
    2.9896    4.6354   13.5694   10.3438    0.4375
    5.1562    5.9062   10.3438    8.6250    0.8125
    0.1250    0.0625    0.4375    0.8125    9.7500
```

1. What operations should be performed ?
2. Calculate the first row.
3. The eigenvalues are as follows : $\lambda_1 = 31.41$, $\lambda_2 = 13.67$, $\lambda_3 = 9.69$, $\lambda_4 = 0.04$, $\lambda_5 = 0.005$. What are the proportions of variance explained by the first 3 axes ?
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Principal Component Analysis : Exercises

Here is the matrix of unit eigenvectors

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V =

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    0.5096   -0.3717   -0.0144    0.5378   -0.5592
    0.4955    0.6469    0.1144    0.4001    0.4035
    0.4753    0.3317    0.0207   -0.6827   -0.4444
    0.0323    0.1168   -0.9917    0.0393    0.0152
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Reminder of the order : Math, Physics, French, Languages, Music

1. Interpret these values.
2. What are the first 3 coordinates of Erwan in this basis ?
3. Interpret the grades in this new space.

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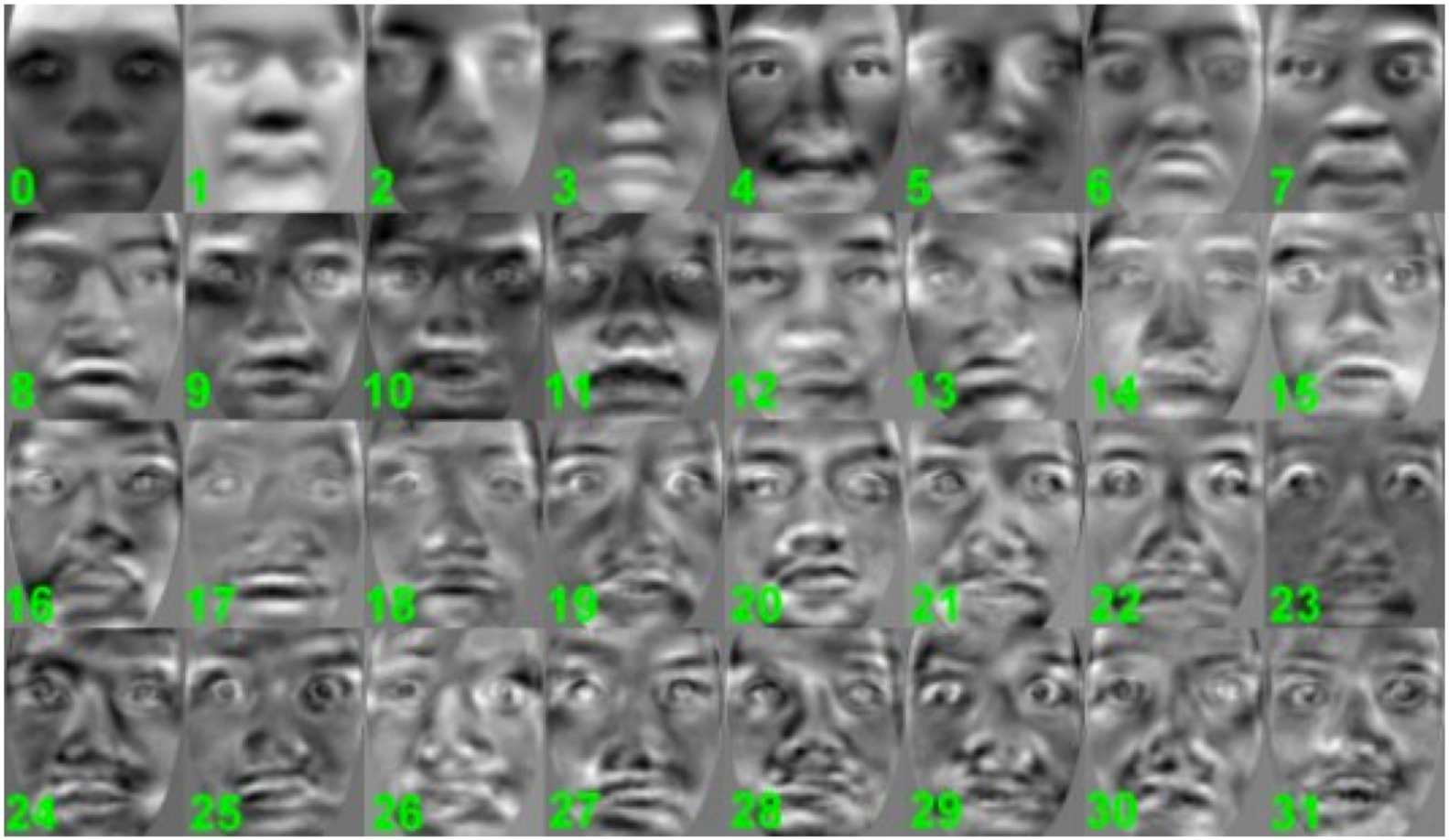
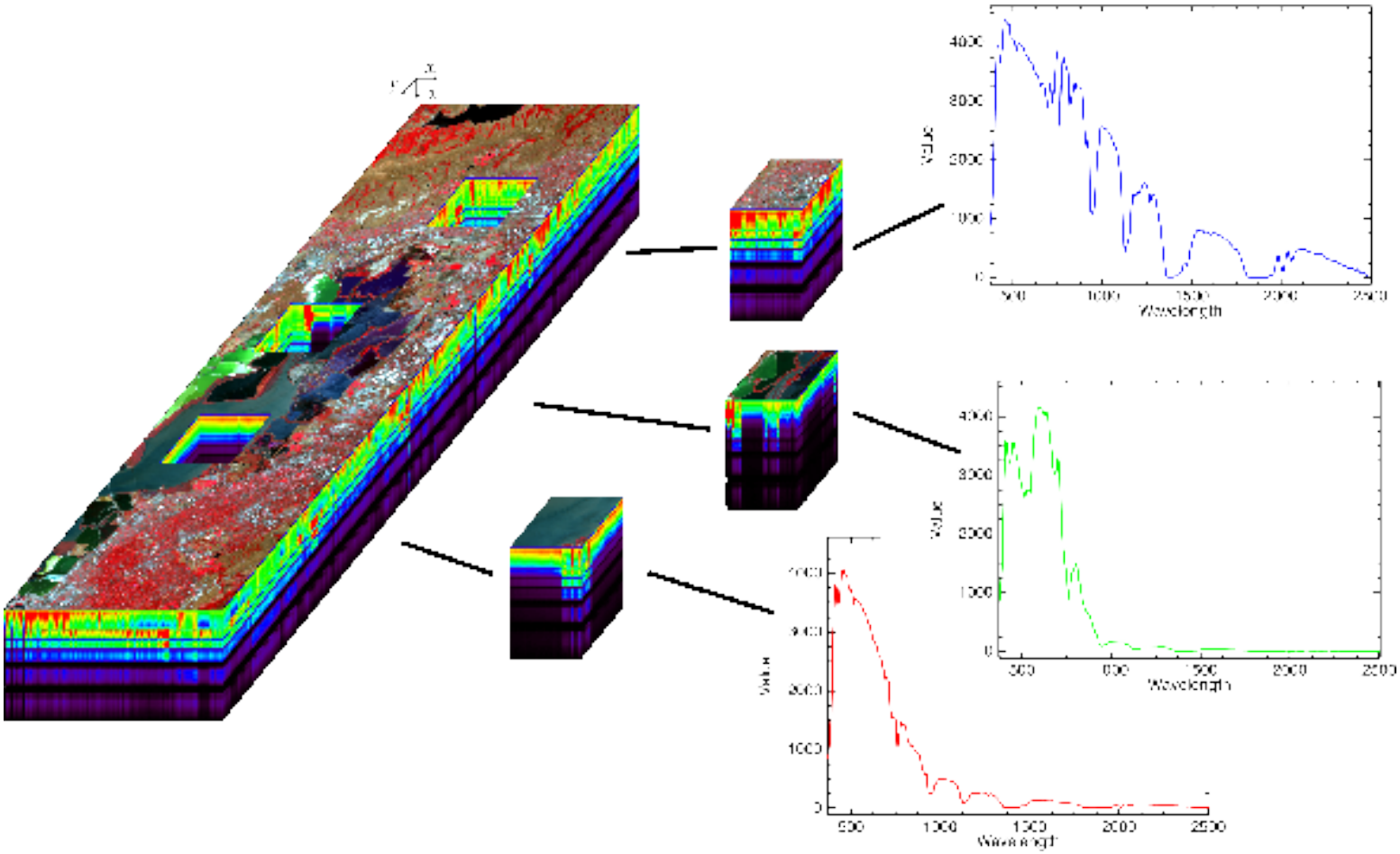
Face Recognition

Creating sets of eigenvectors ("eigenfaces")



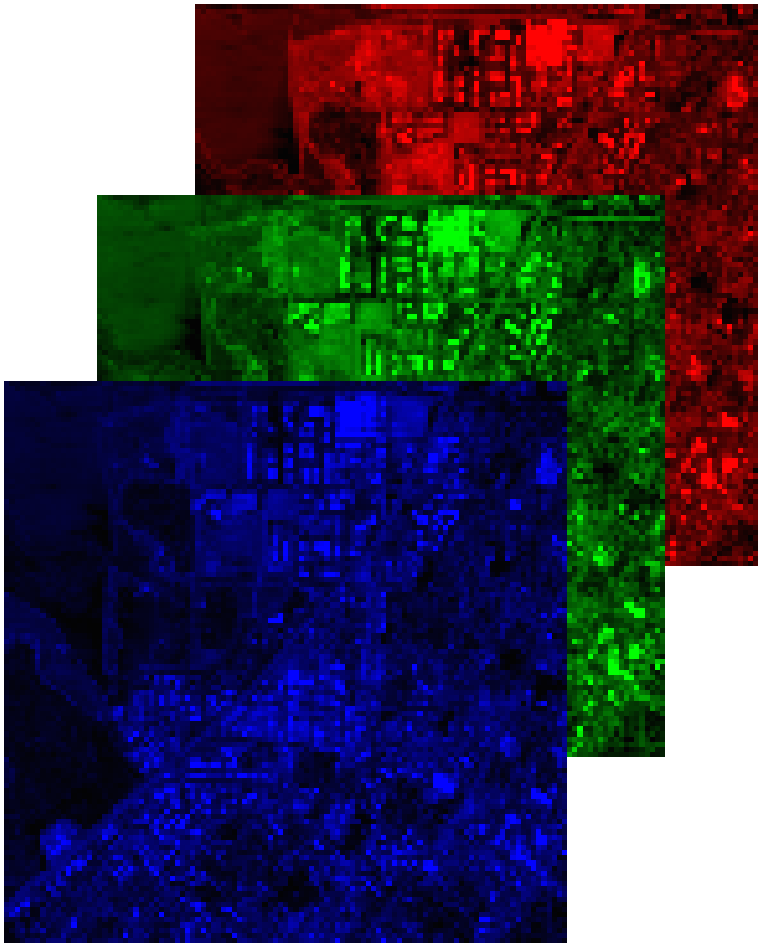
Useful for dimensionality reduction, face recognition, etc.

Hyperspectral Remote Sensing



Hyperspectral Remote Sensing

Color visualization



Interpolation in this Basis

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Instead of interpolating $X_{missing} = MX$, we interpolate

Outline

Locally Linear Embedding

- We have a data matrix X of size $P \times N$ (P measurements i N dimensions).
- Assumption : Locally, the observation cloud X is generated by an affine subspace.
- We seek X' of dimension $M < N$ that accurately represents the structure of X.
  - The neighbors $\mathbf{x}'_j$ of $\mathbf{x}'_i$ in the reduced space must be the same as the neighbors $\mathbf{x}_j$ of $\mathbf{x}_i$ in the original space.

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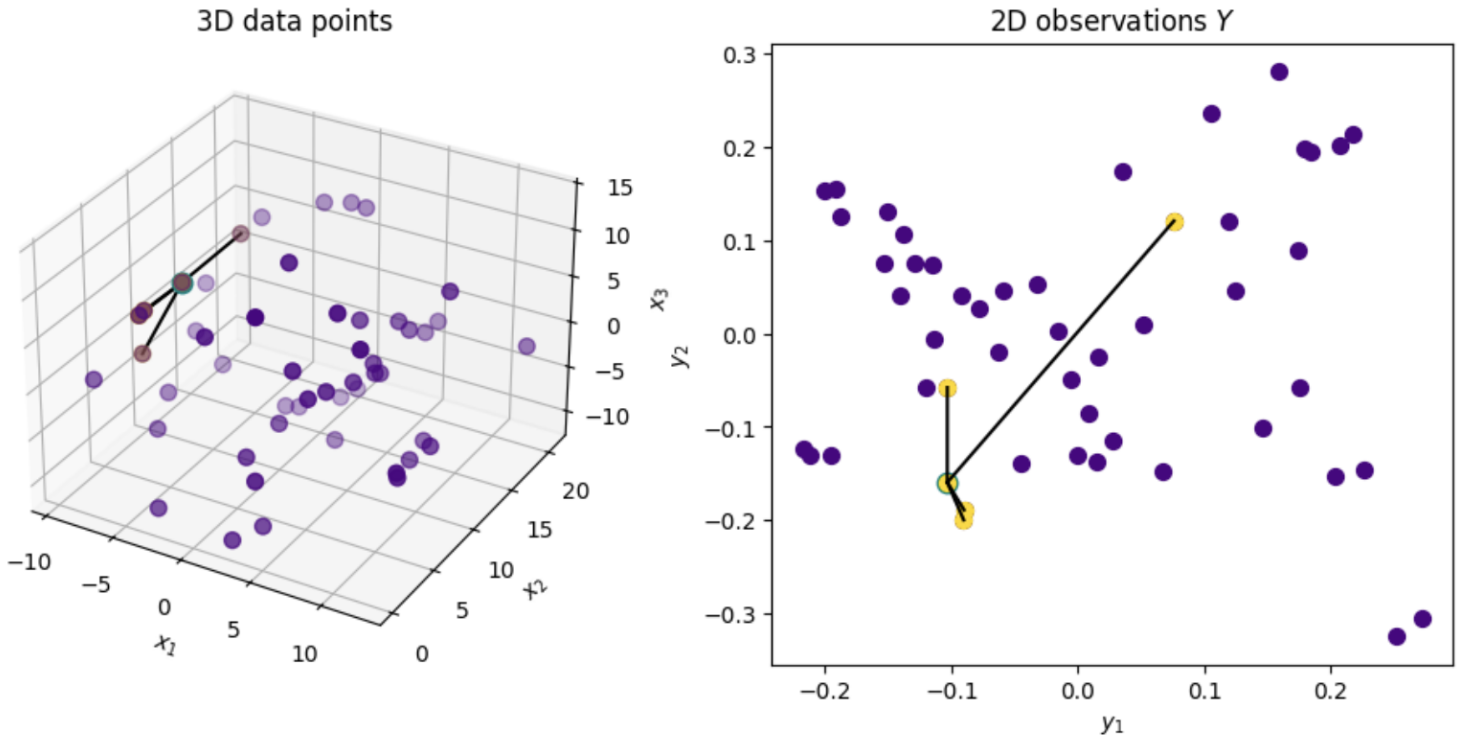
Illustration



Locally Linear Embedding : process

- For each point $\mathbf{x}_i \in \mathbb{R}^N$
  1. Find its neighbors $V_i = \{\mathbf{x}'_1, \mathbf{x}'_2, \dots, \mathbf{x}'_k\}$
  2. Find the best linear combination of $\mathbf{x}_i$ with these neighbors by computing W^* with

$$W^* = \arg\min_W \sum_i \left\| \mathbf{x}_i - \sum_{j \in V_i} w_{ij} \mathbf{x}_j \right\|^2 \text{ s.t. } \sum_j w_{ij} = 1$$

- Find the best reduced data that matches with this linear combination

$$Y^* = \arg\min_Y \sum_i \left\| \mathbf{y}_i - \sum_{j \in V_i} w^*_{ij} \mathbf{y}_j \right\|^2 \text{ with } \mathbf{y}_i \in \mathbb{R}^M$$

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$$Y^* = \arg\min_Y \sum_i \left\| \mathbf{y}_i - \sum_{j \in V_i} w^*_{ij} \mathbf{y}_j \right\|^2 \text{ with } \mathbf{y}_i \in \mathbb{R}^M$$

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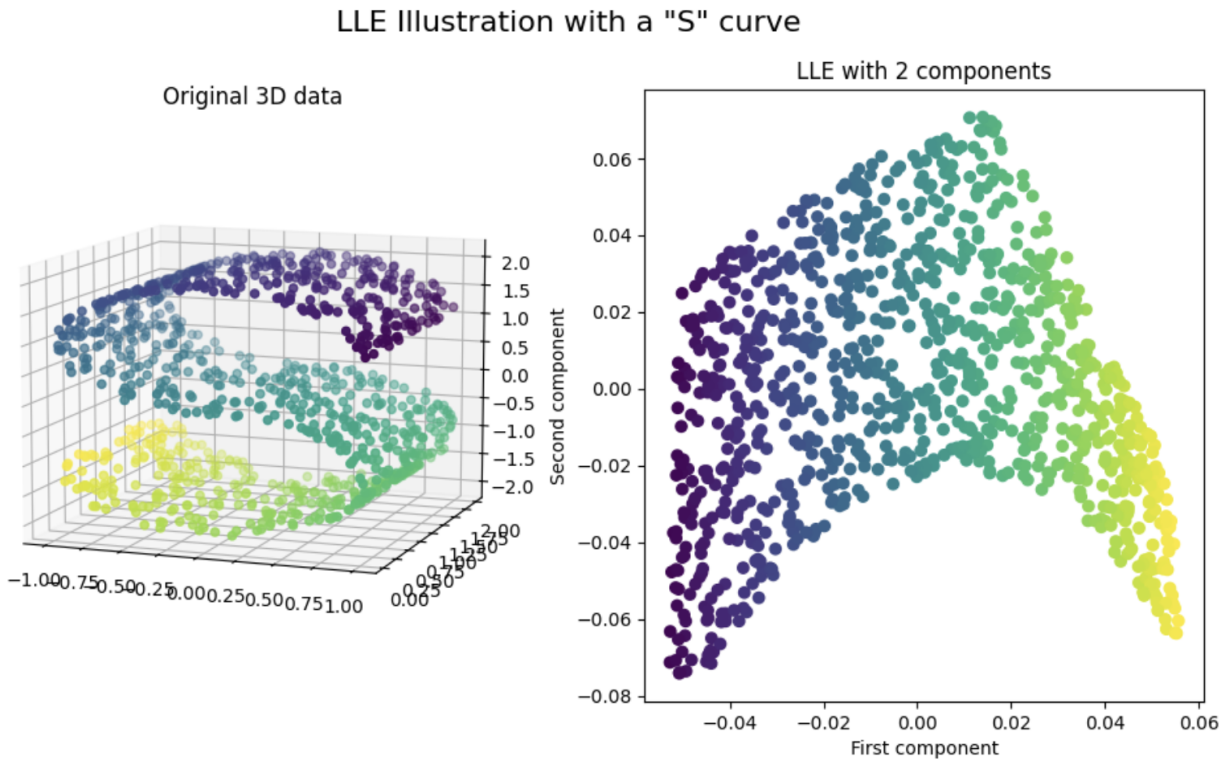

Outline

t-SNE : t-distributed stochastic neighbor embedding

- LLE : Distances
- Distances $\Longrightarrow$ Distributions
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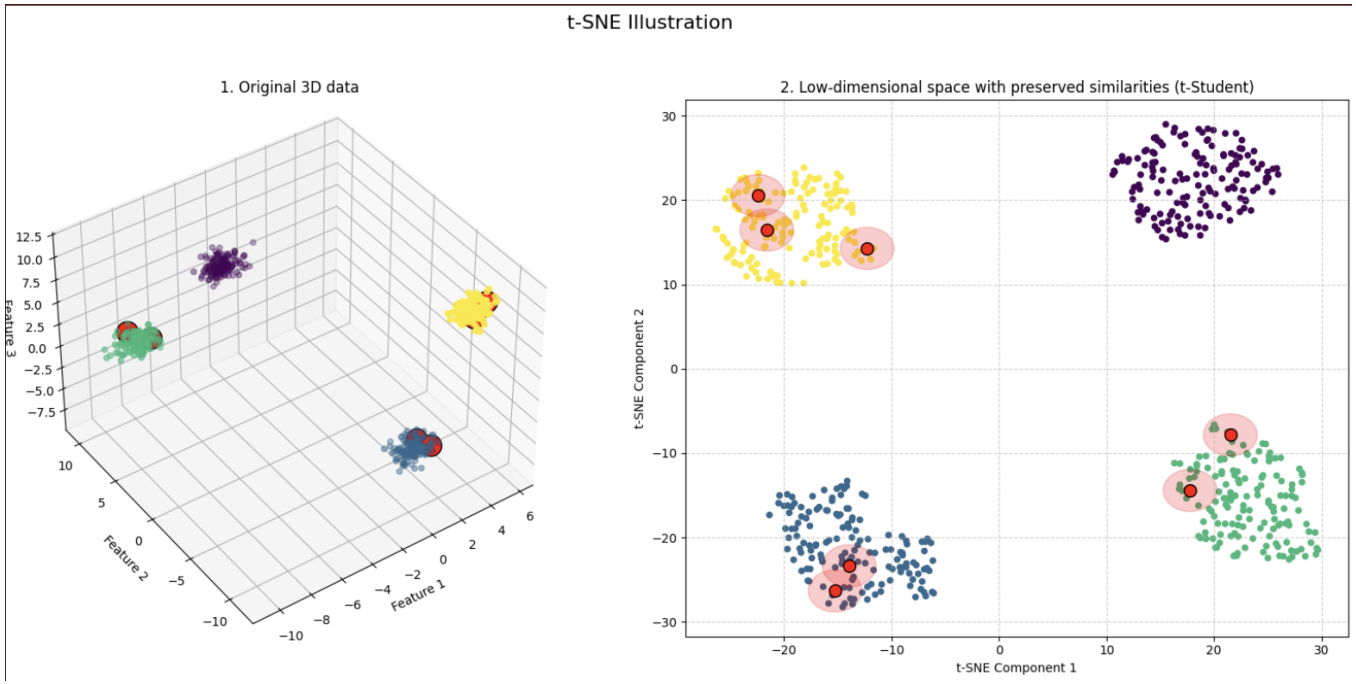

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  - We search for points $\mathbf{y}_i$ in the reduced space for which $p(\mathbf{y}_j|\mathbf{y}_i) \approx p(\mathbf{x}_j|\mathbf{x}_i)$.

t-SNE : t-distributed stochastic neighbor embedding, in practice (1/4)

- Consider a matrix X of size $P \times N$ (P observations $\mathbf{x}_i$, of dimension N).
- To each pair $\mathbf{x}_i, \mathbf{x}_j$, we associate the joint probability $p_{ij} = p_{ji}$ defined by :

$$p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n} \quad \text{with} \quad p_{j|i} = \frac{\exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2/2\sigma_i^2)}{\sum_{k \neq i} \exp(-\|\mathbf{x}_i - \mathbf{x}_k\|^2/2\sigma_i^2)}$$

with the convention that $p_{ii} = 0$ so that $\sum_{i,j} p_{ij} = 1$.

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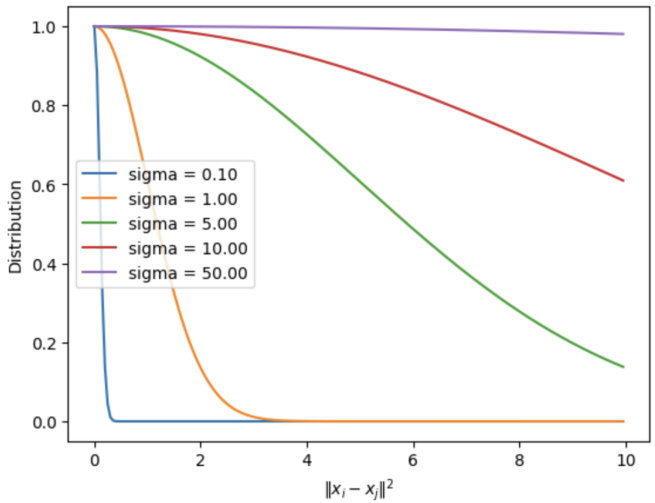
- [σ] is chosen based on the desired **perplexity** ($\sim$ average number of neighbors).



t-SNE : t-distributed stochastic neighbor embedding, in practice (2/4)

Similarity in the low-dimensional space (or embedding space)

- The objective of t-SNE is to obtain a low-dimensional matrix $\mathbf{Y}$ of dimension $P \times M$, where $M < N$, such that the similarities q_{ij} approximate the p_{ij}.
- For $\mathbf{Y}$, the similarity is defined using a Student's t-distribution with 1 degree of freedom (also known as the Cauchy distribution) :

$$q_{ij} = \frac{(1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-1}}{\sum_{k \neq l}(1 + \|\mathbf{y}_k - \mathbf{y}_l\|^2)^{-1}}$$

with the convention, here again, that $q_{ii} = 0$.

t-SNE : t-distributed stochastic neighbor embedding, in practice (3/4)

Gaussian vs. Student's t-distribution

- **High-Dimensional Space : Gaussian Distribution**
  - Thin tails : probability drops off very quickly with distance.
  - $\Longrightarrow$ Only immediate neighbors are considered important.
  - **Goal :** To accurately capture the *local structure*.
- **Low-Dimensional Space : Student's t-distribution**
  - Heavy tails : probability decreases much more slowly.
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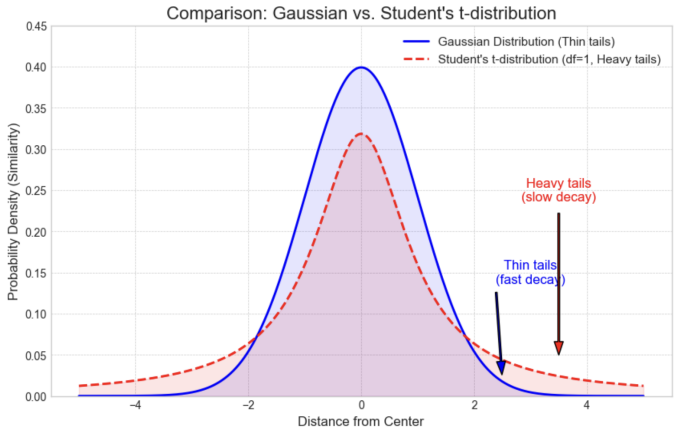
  - Solves the **crowding problem** for clear, separated clusters.



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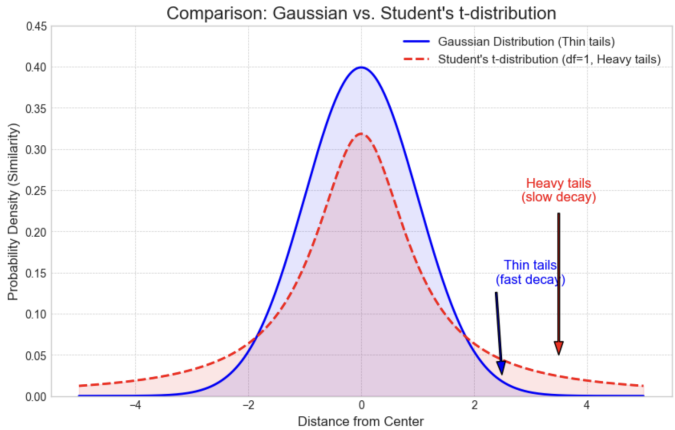

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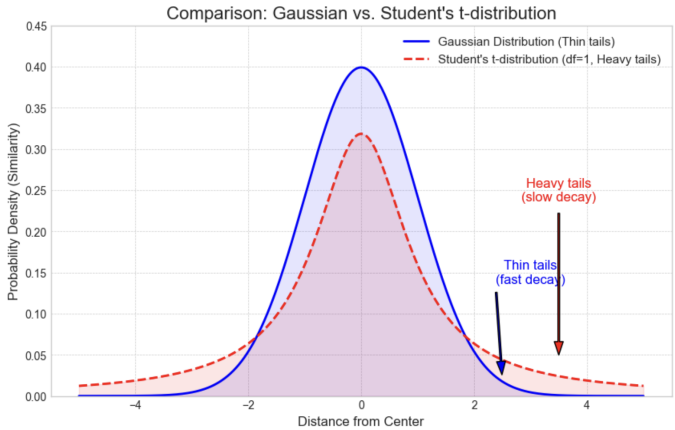

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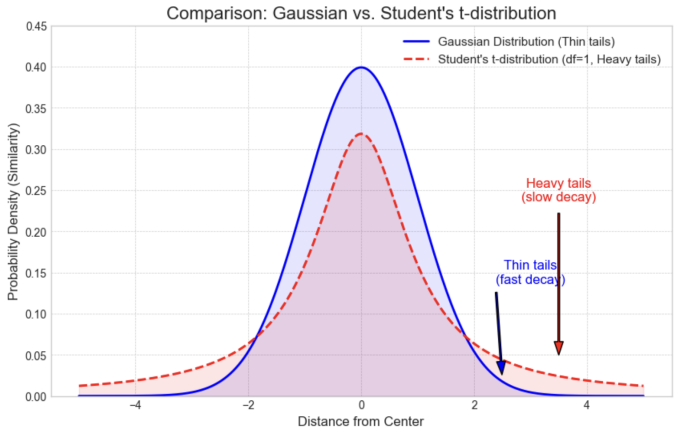

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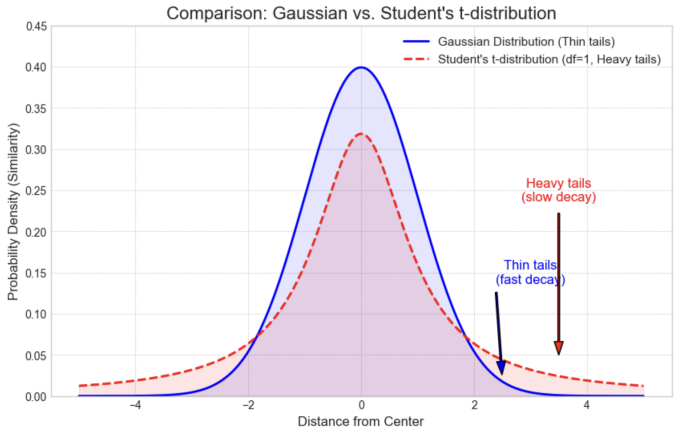

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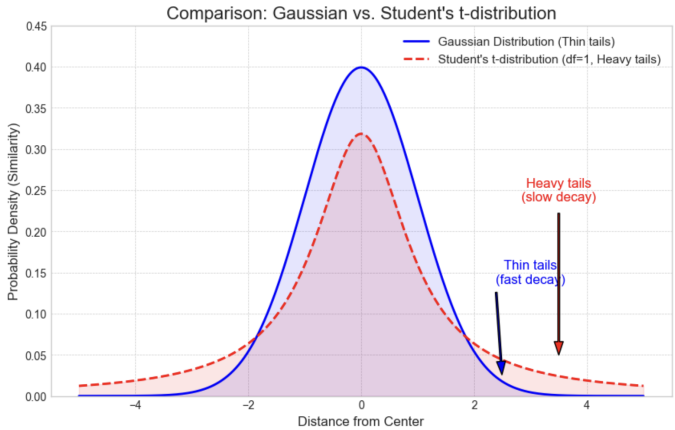

t-SNE : t-distributed stochastic neighbor embedding, in practice (3/3)

- A measure of dissimilarity between distributions is the **Kullback-Leibler divergence** :

$$L_{t-\text{SNE}} = \sum_i D_{\text{KL}}(P\|Q) = \sum_i \sum_j p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

- To minimize the differences between the q_{ij} and the p_{ij}, it is sufficient to minimize $L_{t-\text{SNE}}$.

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- Main parameters
  1. Perplexity `perplexity`
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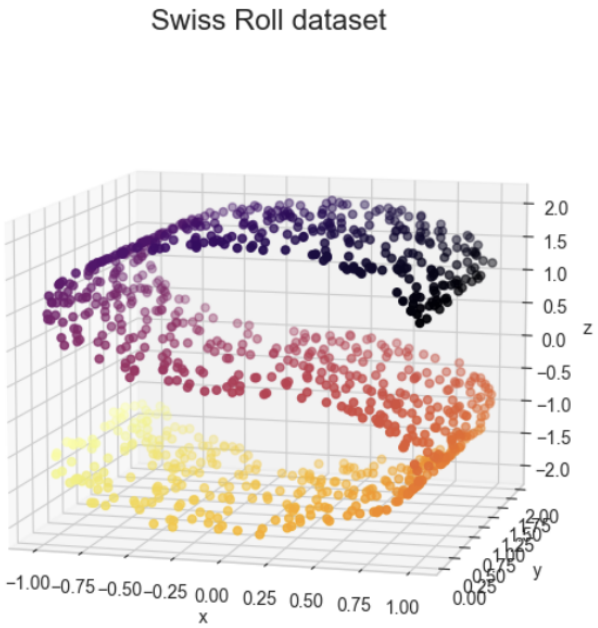

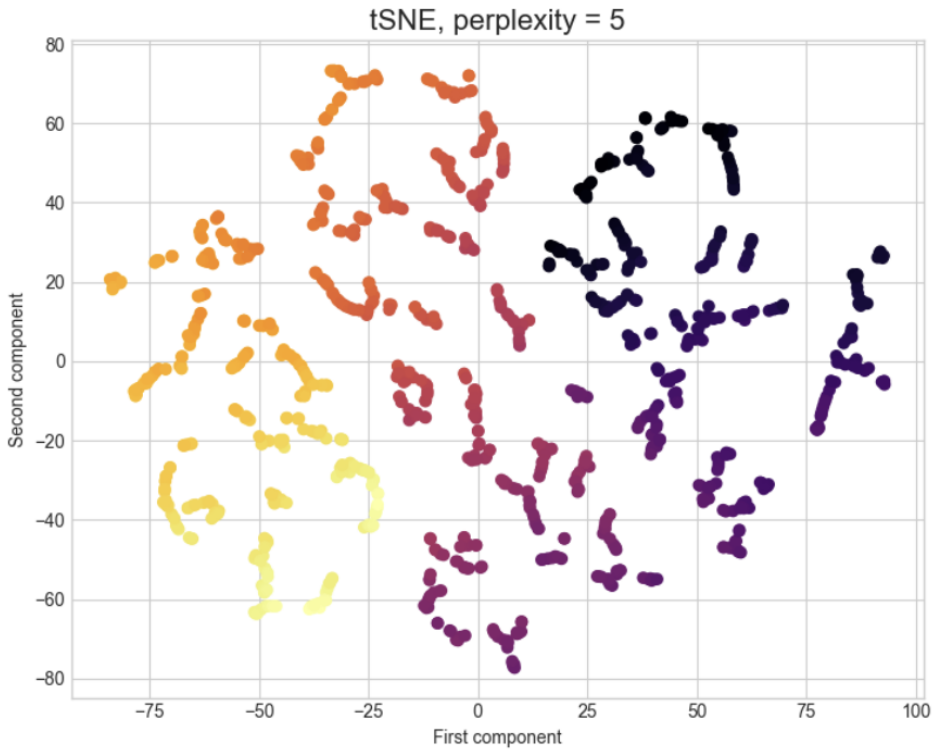

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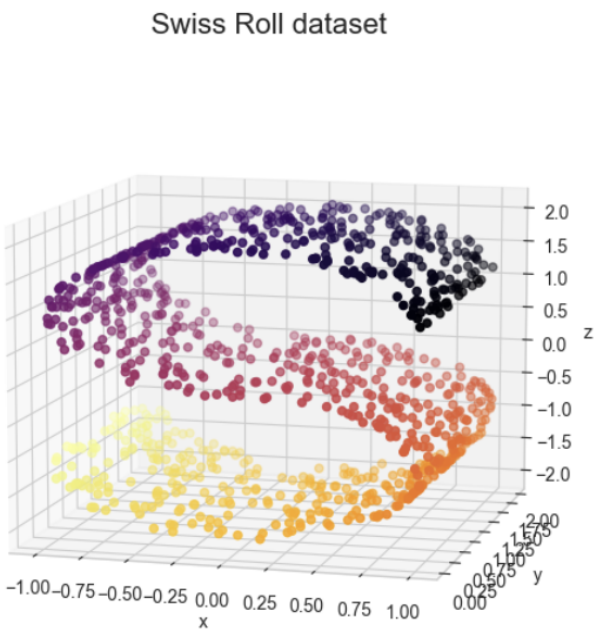

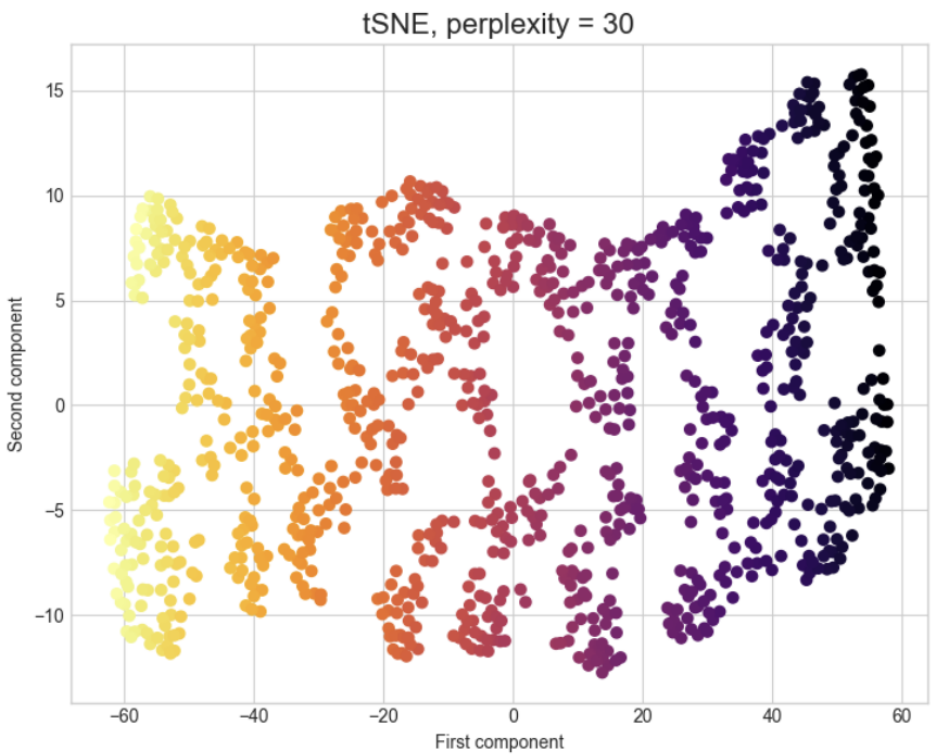

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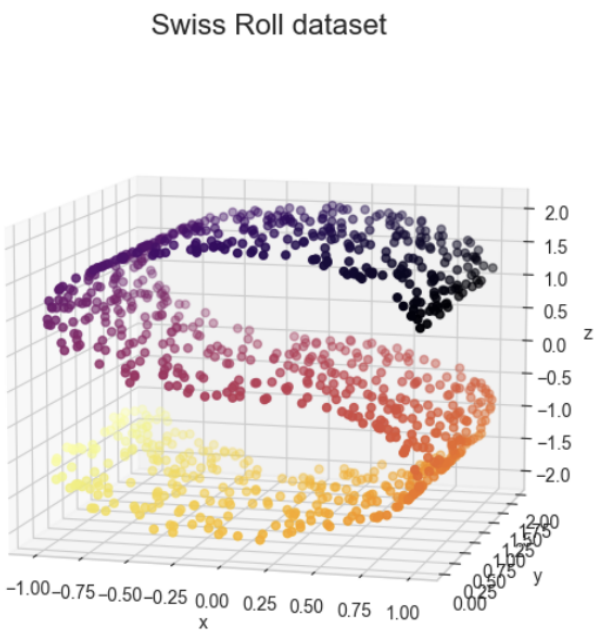

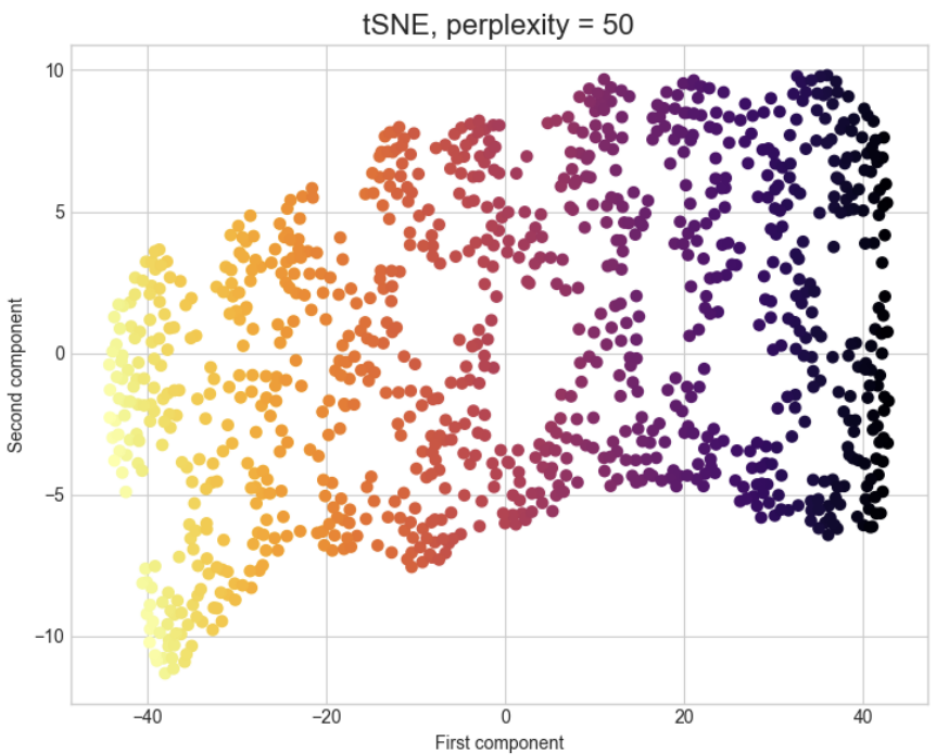

LLE vs. t-SNE : Key Differences

Locally Linear Embedding (LLE)

- **Principle :** Geometric & Deterministic.
- **Assumption :** Assumes the data lies on a manifold that is *locally linear*.
- **Mechanism :** Preserves the **linear reconstruction weights** of each point from its nearest neighbors.
- **Best Use Case :** "Unrolling" single, continuous, and smooth manifolds (e.g., a Swiss Roll).

t-SNE

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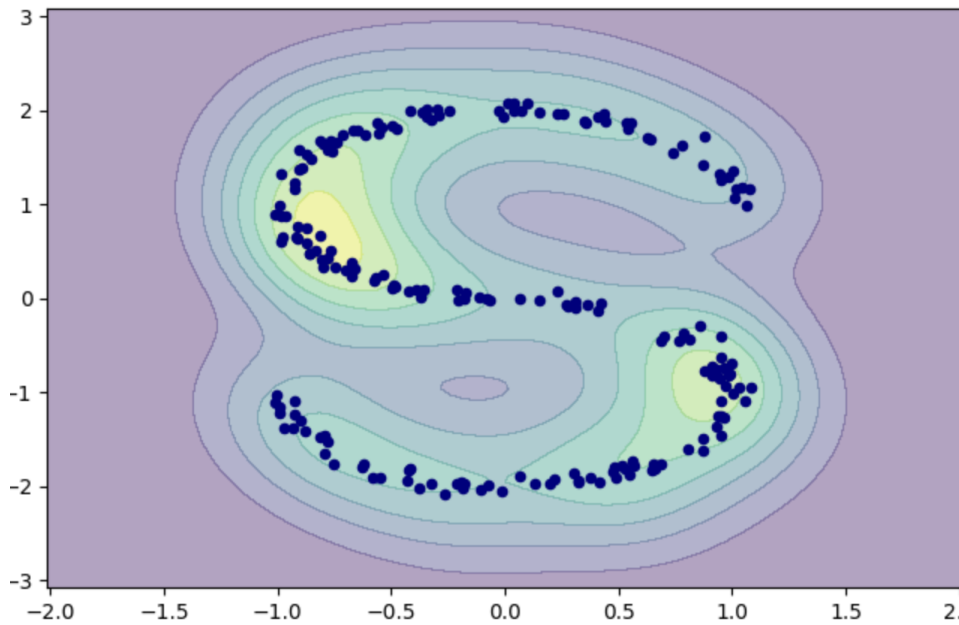
UMAP : Uniform Manifold Approximation & Projection

General Idea

- Find a low-dimensional representation that has the same **topological structure** as the original data.



Main Steps

1. Define an appropriate / adaptive similarity metric.
2. Construct a **similarity graph** based on these similarities in the high-D space.
3. Find a low-dimensional embedding that has the most similar graph structure possible.

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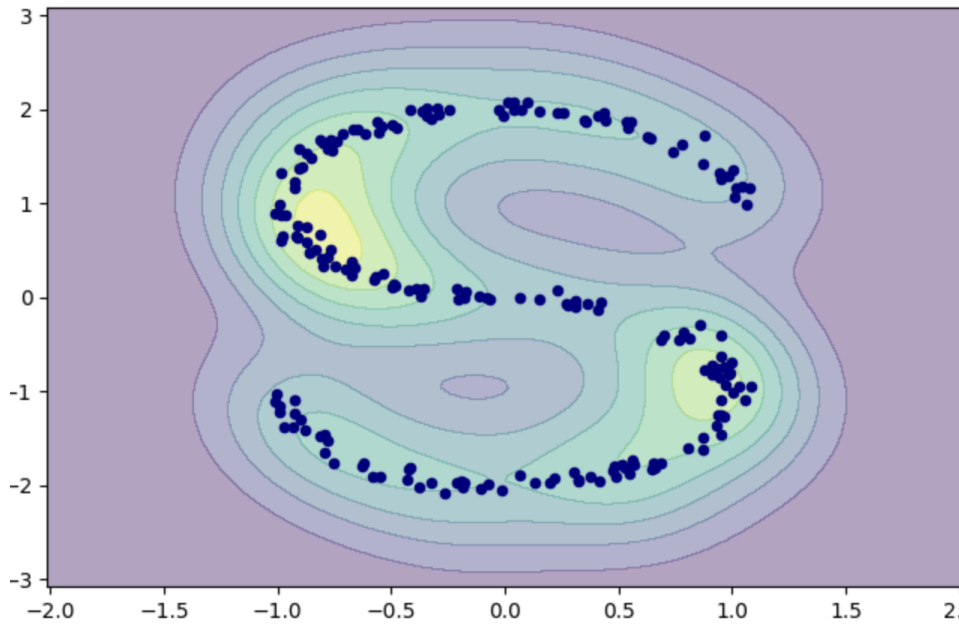

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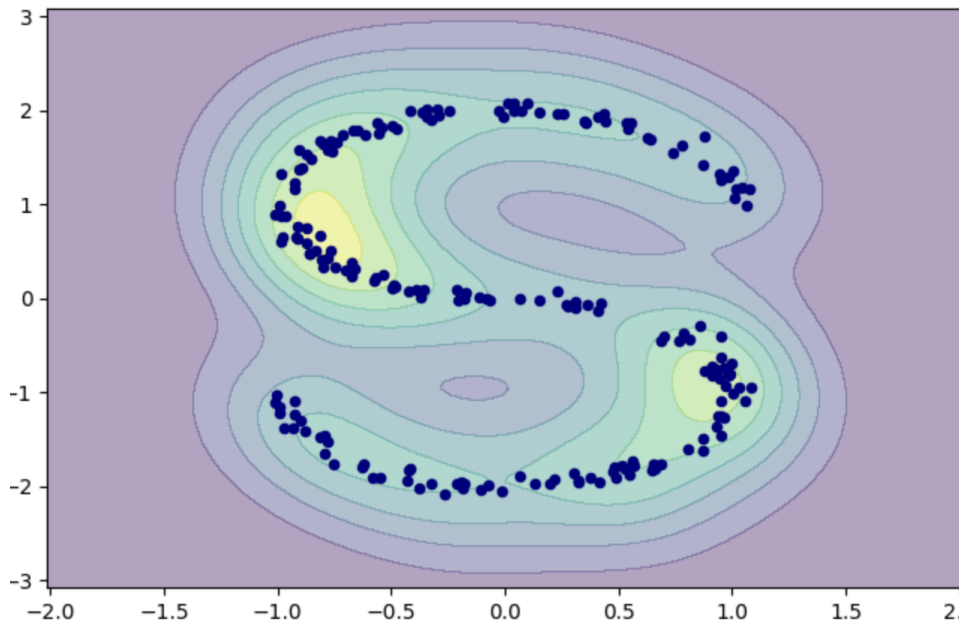

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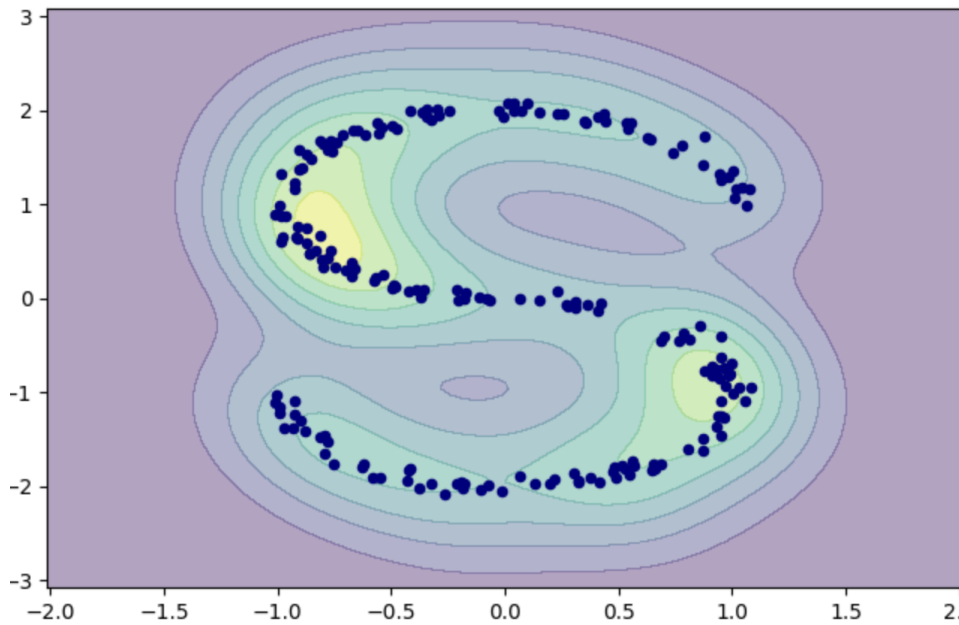
- Find a low-dimensional representation that has the same **topological structure** as the original data.



Main Steps

1. Define an appropriate / adaptive similarity metric.
2. Construct a **similarity graph** based on these similarities in the high-D space.
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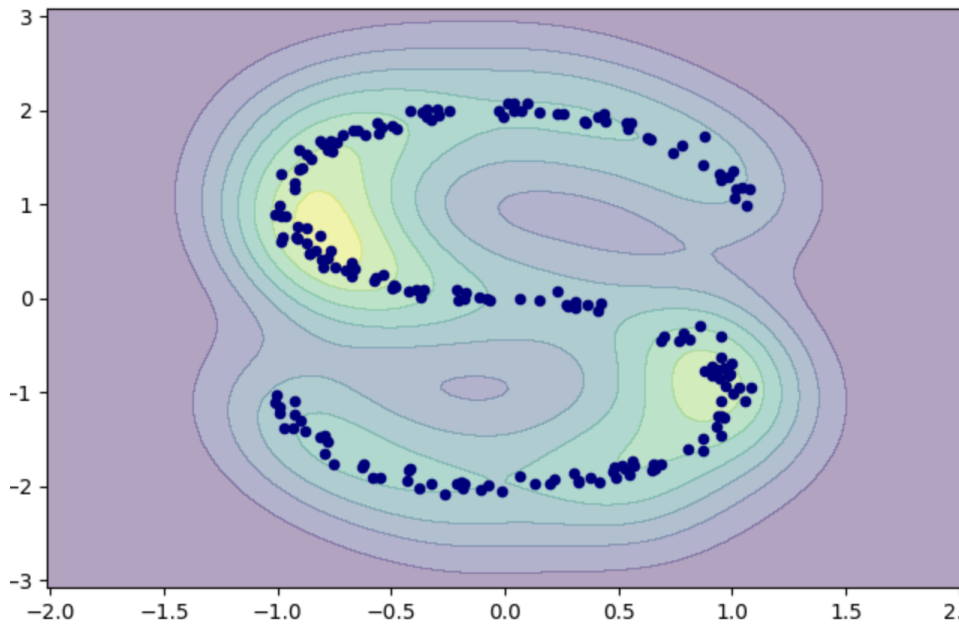

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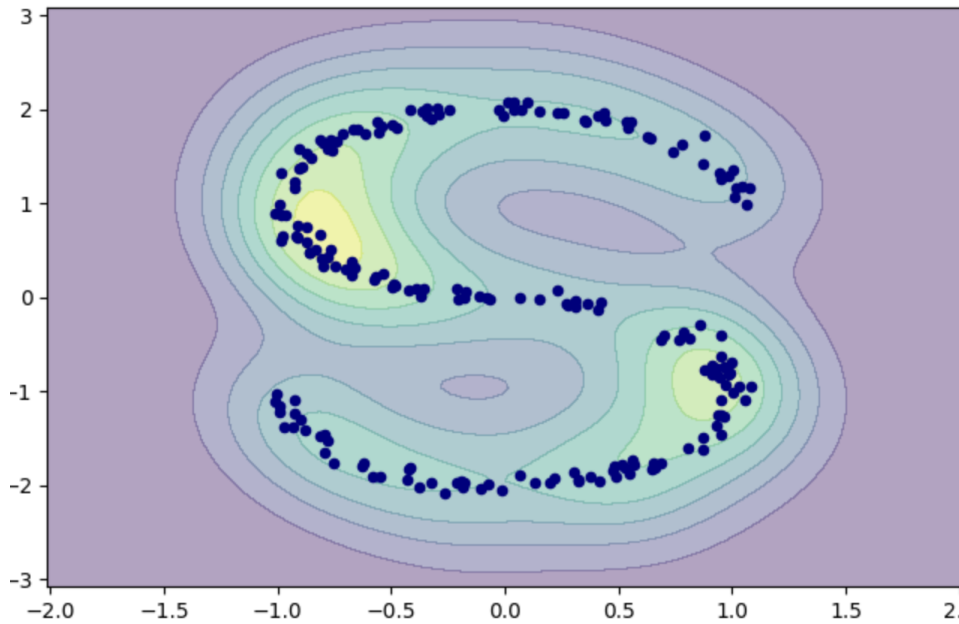

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Major Differences from t-SNE.

- **Adapts to Local Density :**
  - Uses a variable notion of similarity depending on the data density.
  - This allows it to better handle clusters with **varying densities** (**varying perplexity**).
- **More Flexible Similarities :**
  - Uses a broader family of similarity functions in the low-dimensional space.
- **Better Global Structure :**
  - Preserve the local/global data structure better than t-SNE

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UMAP : Adaptive Similarity in the Original space

- UMAP defines an adaptive similarity that varies with the local data density :

$$p_{i|j} = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2 - \rho_i}{\sigma_i}\right)$$

where ρ_i is the distance from $\mathbf{x}_i$ to its nearest neighbor.

- The bandwidth σ_i is set such that :

$$\sum_{j=1}^{k} \exp\left(-\frac{\max(0, \|\mathbf{x}_i - \mathbf{x}_j\| - \rho_i)}{\sigma_i}\right) = \log_2(k)$$

where k is the parameter for the number of nearest neighbors to consider.

$\Longrightarrow$ we measure only distances higher than nearest neighbor

- $\log_2(k)$ term : every point must distribute among its k nearest neighbors

$\Longrightarrow$ Forcing the algorithm to find an adaptive local scale σ_i to meet this target.

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Technical issues :

- For two points $\mathbf{x}_i$ and $\mathbf{x}_j$, the joint similarity p_{ij} must be symmetric ($p_{ij} = p_{ji}$). In UMAP, this is achieved by :

$$p_{ij} = p_{j|i} + p_{i|j} - p_{j|i} \cdot p_{i|j}$$

  - Symmetrization is necessary because $\rho_i \neq \rho_j$ (and thus $\sigma_i \neq \sigma_j$).
  - As a reminder, t-SNE uses a different symmetrization : $p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$.

Similarity in the Embedding Space

- Best curve

$$f(d) = \begin{cases} 1 & \text{if } d \leq \text{min\_dist} \\ e^{-(d - \text{min\_dist})} & \text{if } d > \text{min\_dist} \end{cases}$$

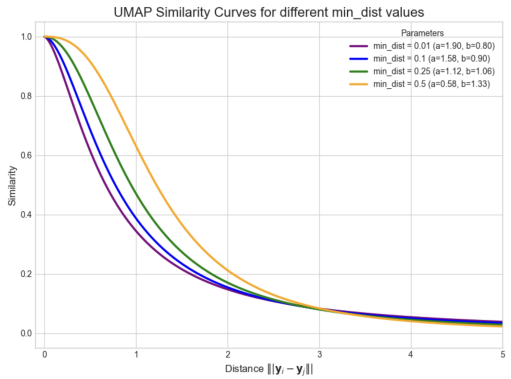
where $d = \|\mathbf{y}_i - \mathbf{y}_j\|$ and **min_dist** is the minimum allowed distance between two points in the embedding space.

- Similarity in the embedding space : inspired by the Student's t-distribution :

$$q_{ij} = \frac{1}{1 + a\|\mathbf{y}_i - \mathbf{y}_j\|^{2b}}$$

$\Longrightarrow$ **Heavy tail** to avoid the crowding problem.

- Parameters a and b are chosen automatically such that this curve, q, provides the **best possible fit** to the target curve, $f(d)$.



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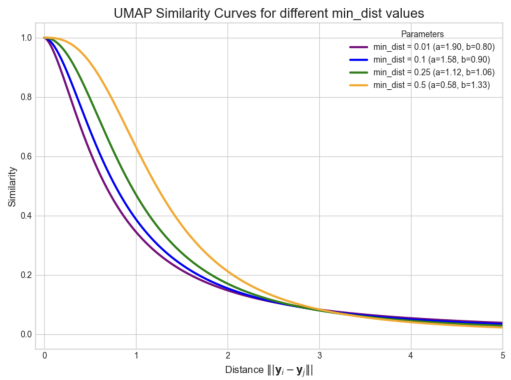

Illustration

- Main parameters
  1. Number of components `n_components`
  2. Number of neighbors `n_neighbors` (The most similar parameter to t-SNE's perplexity)
  3. Minimal distance `min_dist`

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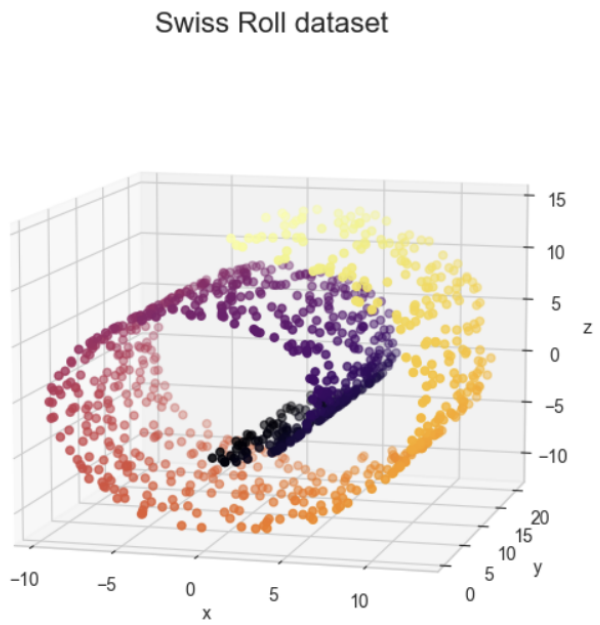

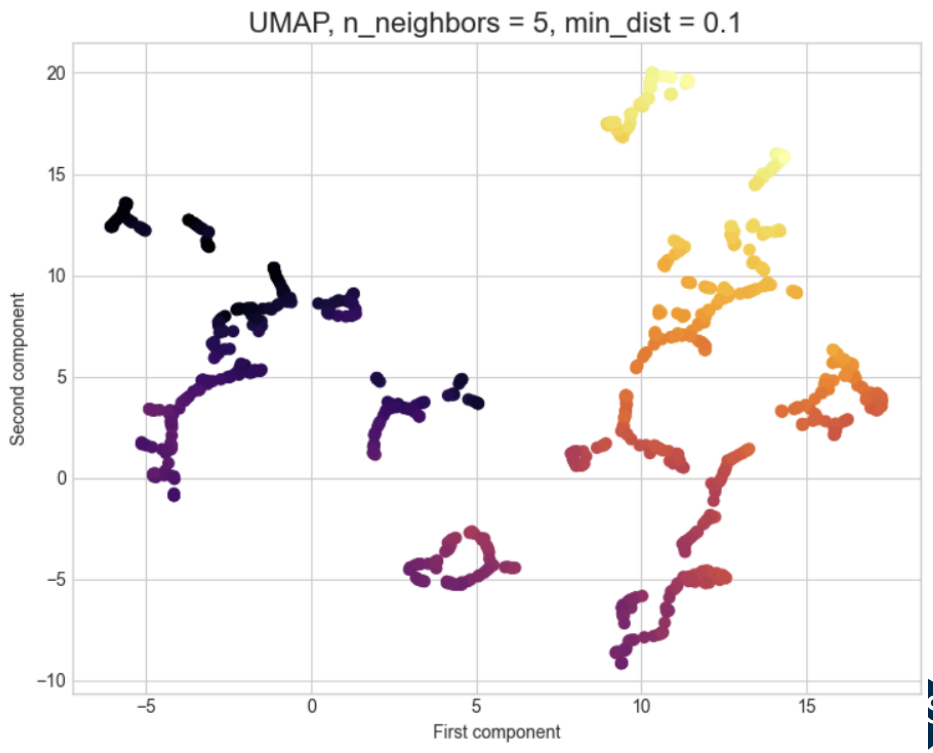

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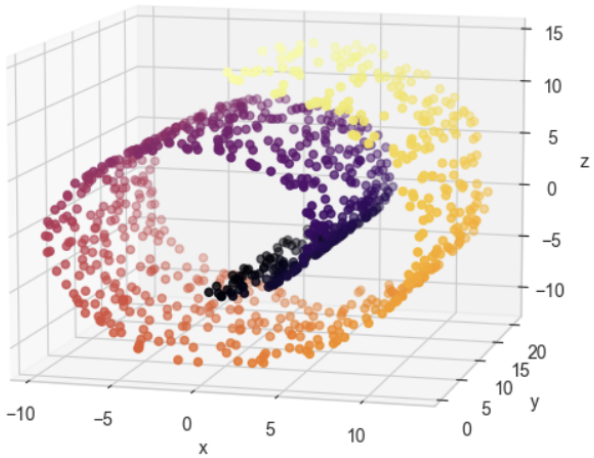

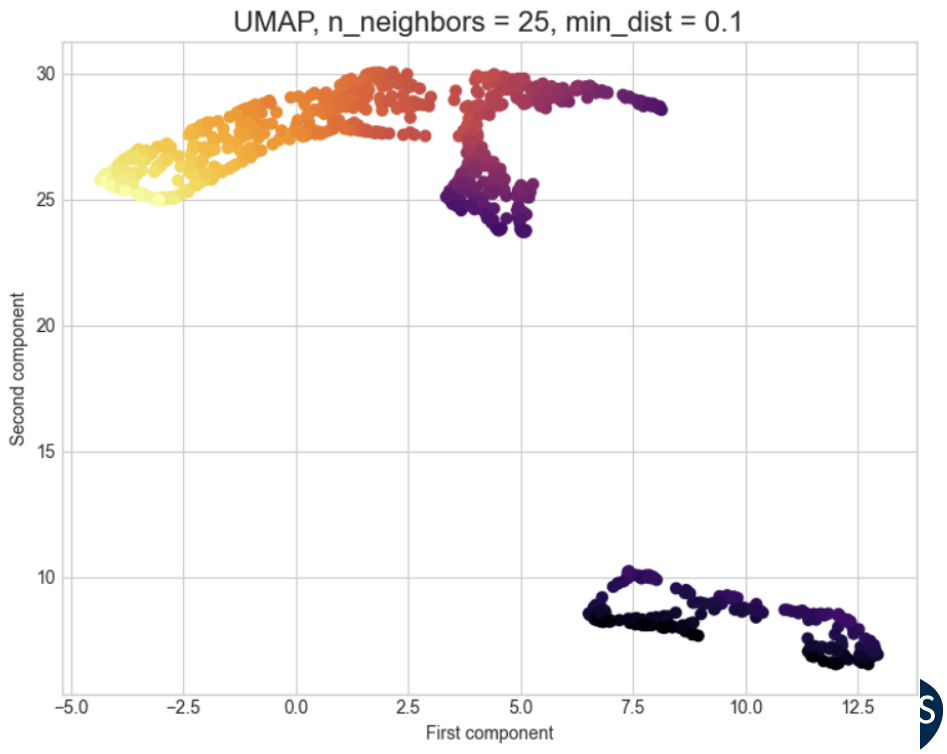

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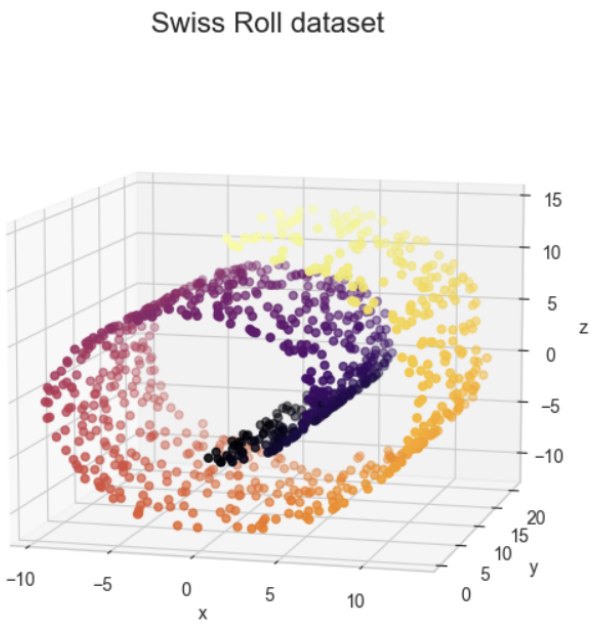

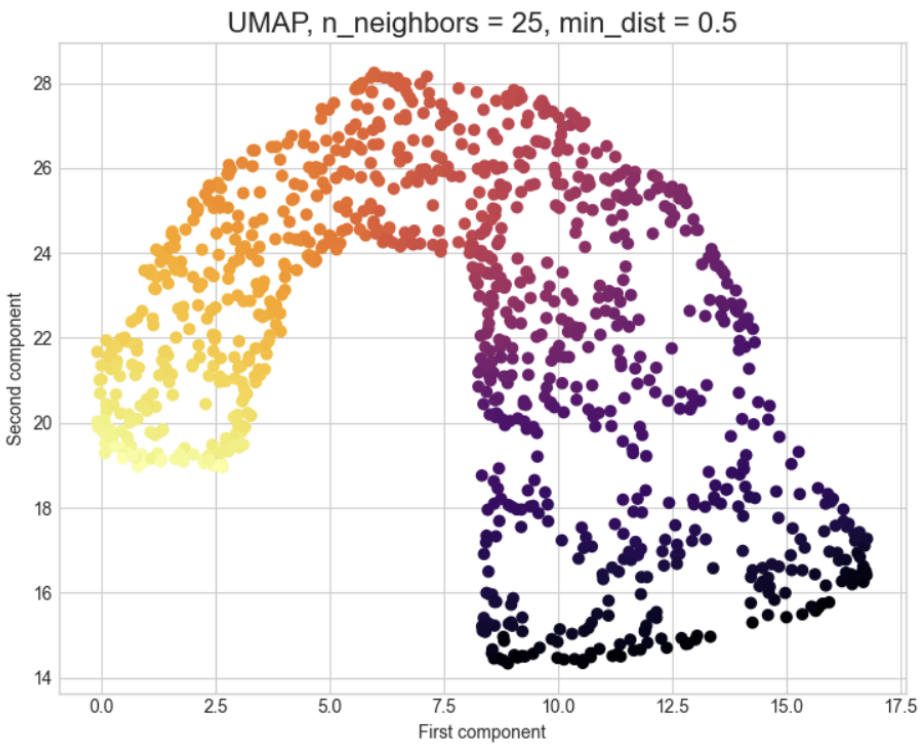

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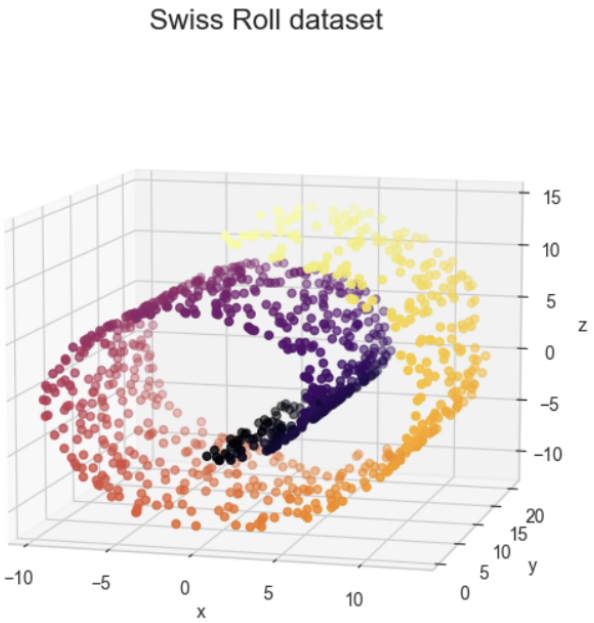

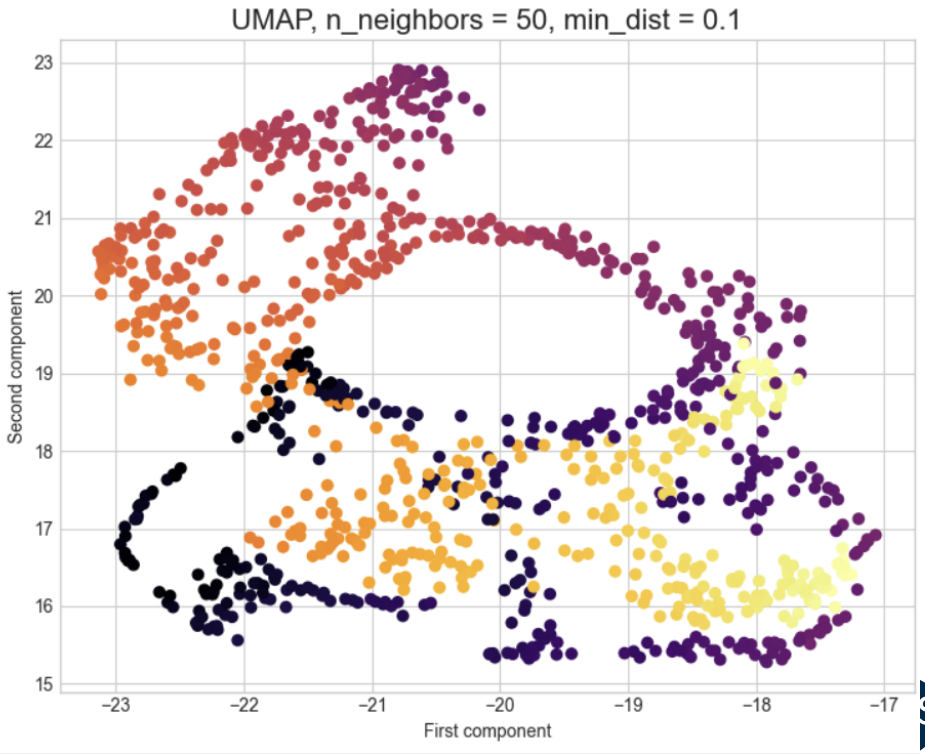

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