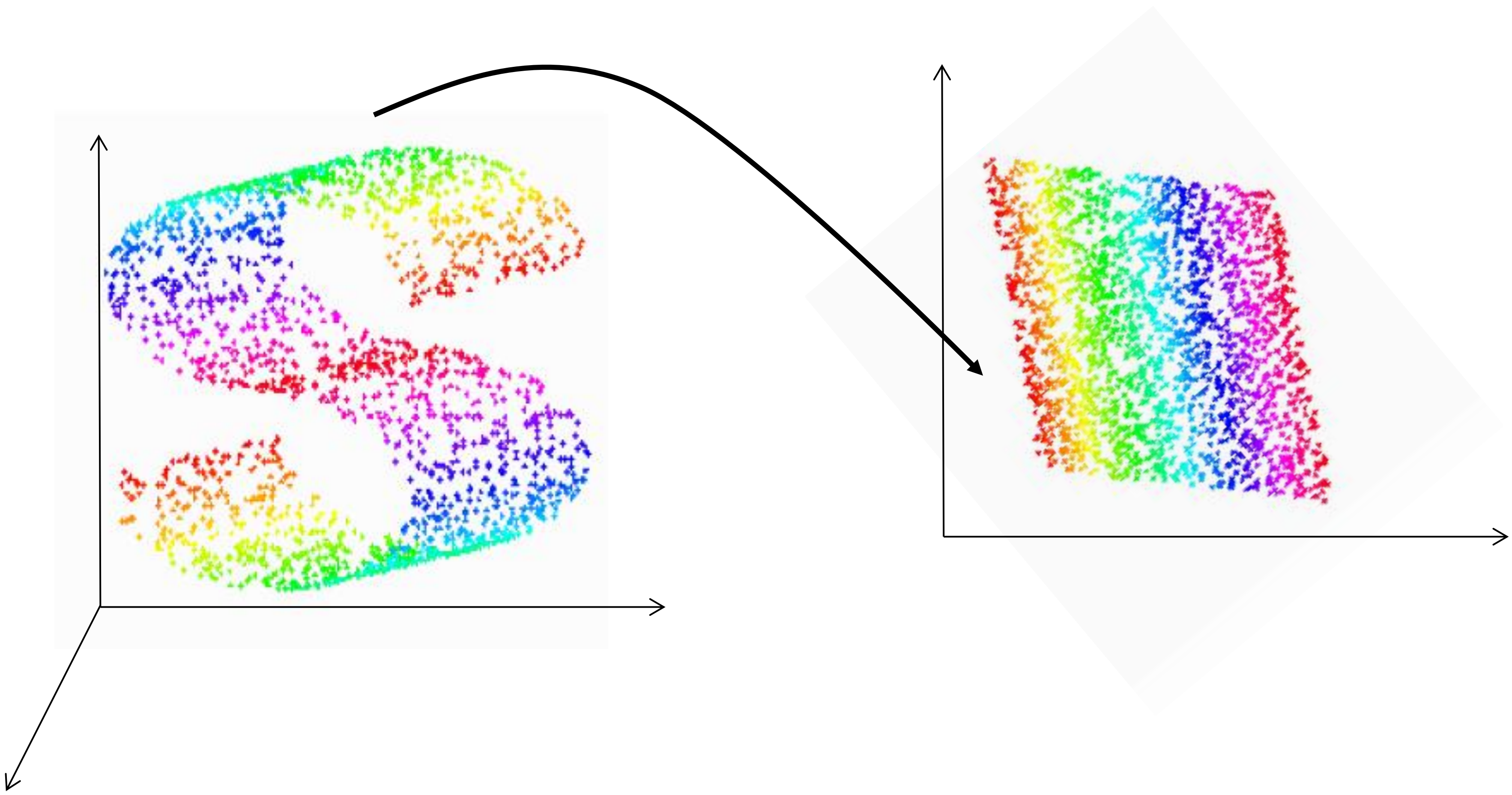
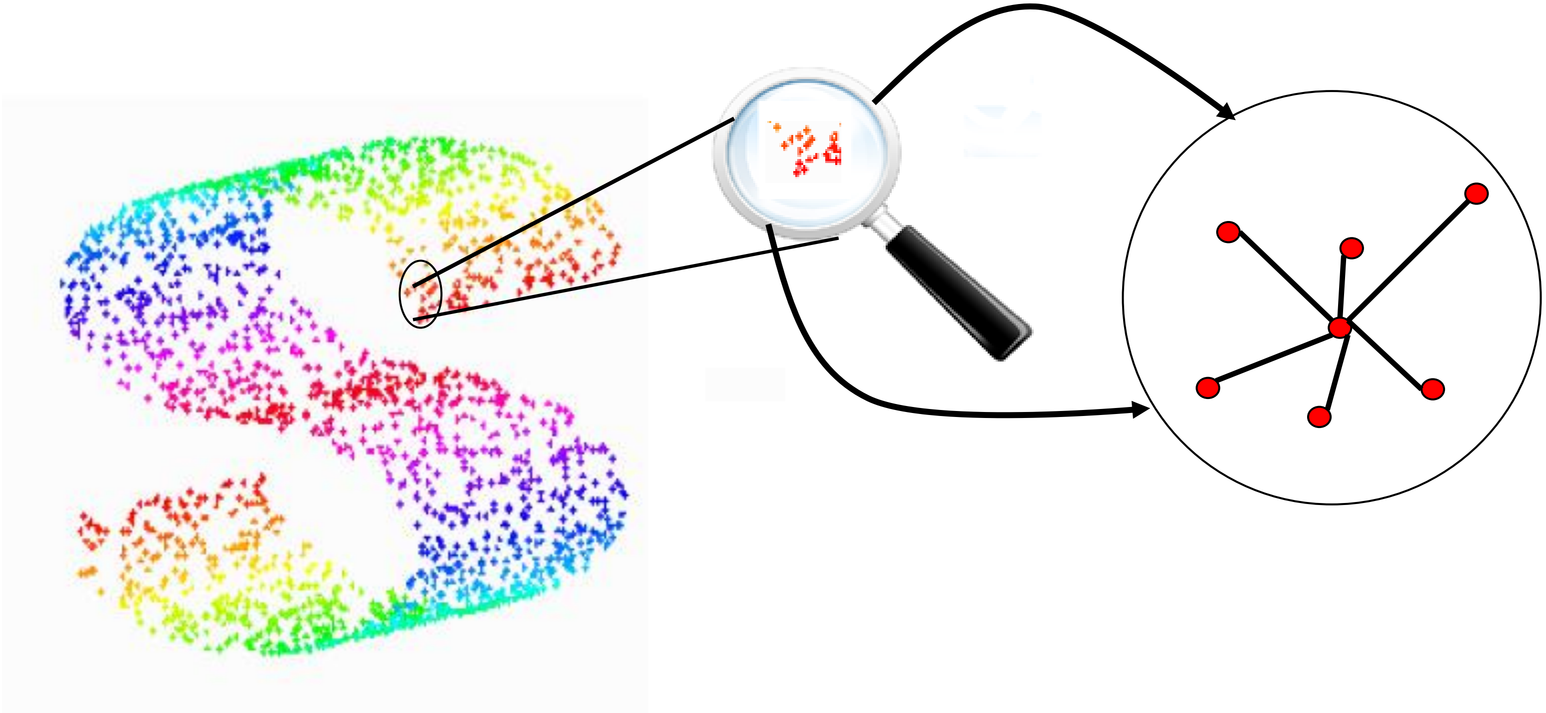
Locality preserving latent spaces



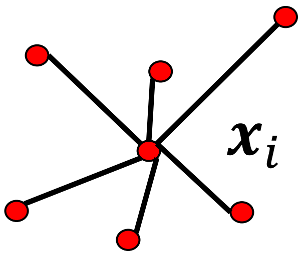
Locality preserving latent spaces

We want to find a latent space that preserves the local structure



Locality preserving latent spaces

How can we define the local structure?



A k-neighbourhood (k-closest points to $\boldsymbol{x}_i$)

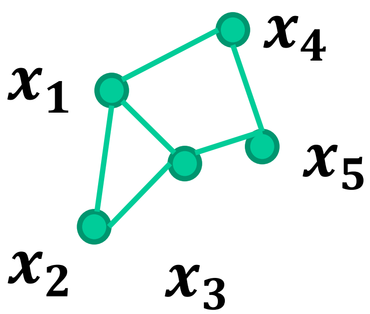
$$c_i{}^k = \{\boldsymbol{x}_\mathrm{j} : \boldsymbol{x}_\mathrm{j} \text{ in } k \text{ closest according } \left|\left|\boldsymbol{x}_i - \boldsymbol{x}_j\right|\right|^2\}$$

$$\{c_1{}^k, \dots, c_N{}^k\}$$

$$\min \frac{1}{2} \sum_{i=1}^{N} \sum_{x_j \in c_i{}^k} (y_i - y_j)^2 = \min \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} s_{ij} (y_i - y_j)^2$$

$\boldsymbol{S}$ is the connectivity matrix, i.e. $s_{ij} = 1$ iff $\boldsymbol{x}_j \in c_i{}^k$ and zero elsewhere

Making the graph



$$s_{ij} = 1 \text{ iff } x_j \in c_i^{\,k}$$

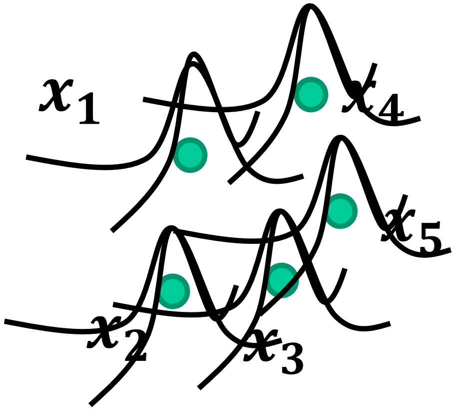
$$\boldsymbol{S} = \begin{array}{c|ccccc} & \boldsymbol{x}_1 & \boldsymbol{x}_2 & \boldsymbol{x}_3 & \boldsymbol{x}_4 & \boldsymbol{x}_5 \\ \boldsymbol{x}_1 & 0 & 1 & 1 & 0 & 0 \\ \boldsymbol{x}_2 & 1 & 0 & 1 & 0 & 0 \\ \boldsymbol{x}_3 & 1 & 0 & 0 & 0 & 1 \\ \boldsymbol{x}_4 & 1 & 0 & 0 & 0 & 1 \\ \boldsymbol{x}_5 & 0 & 0 & 1 & 1 & 0 \end{array}$$

$$c_1 = \{\boldsymbol{x}_2, \boldsymbol{x}_3\}$$
$$c_2 = \{\boldsymbol{x}_1, \boldsymbol{x}_3\}$$
$$c_3 = \{\boldsymbol{x}_1, \boldsymbol{x}_5\}$$
$$c_4 = \{\boldsymbol{x}_1, \boldsymbol{x}_5\}$$
$$c_5 = \{\boldsymbol{x}_4, \boldsymbol{x}_3\}$$

$$s_{ij} = 1 \text{ iff } x_j \in c_i^{\,k} \text{ or } x_i \in c_j^{\,k}$$

$$\boldsymbol{S} = \begin{array}{c|ccccc} & \boldsymbol{x}_1 & \boldsymbol{x}_2 & \boldsymbol{x}_3 & \boldsymbol{x}_4 & \boldsymbol{x}_5 \\ \boldsymbol{x}_1 & 0 & 1 & 1 & 1 & 0 \\ \boldsymbol{x}_2 & 1 & 0 & 1 & 0 & 0 \\ \boldsymbol{x}_3 & 1 & 1 & 0 & 0 & 1 \\ \boldsymbol{x}_4 & 1 & 0 & 0 & 0 & 1 \\ \boldsymbol{x}_5 & 0 & 0 & 1 & 1 & 0 \end{array}$$

Making the graph



$$s_{ij} = e^{-\frac{||x_i - x_j||^2}{t}} \text{ iff } \boldsymbol{x}_i \in c_j{}^k \text{or } \boldsymbol{x}_j \in c_i{}^k$$

or

$$s_{ij} = e^{-\frac{||x_i - x_j||^2}{t}}$$

Formulating the problem

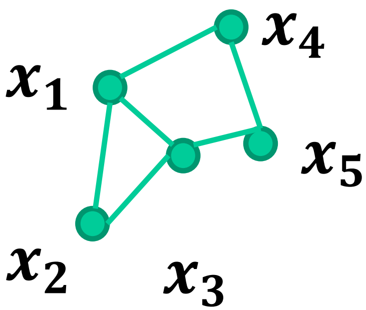
$$\frac{1}{2}\sum_{j=1}^{N}\sum_{i=1}^{N} s_{ij}(y_i - y_j)^2 = \underbrace{\frac{1}{2}\sum_{i=1}^{N}\underbrace{\left(\sum_{j=1}^{N} s_{ij}\right)}_{d_{ii}} {y_i}^2}_{\mathbf{y}^T\boldsymbol{D}\mathbf{y}} - \underbrace{\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} s_{ij} y_i y_j}_{\mathbf{y}^T\boldsymbol{S}\boldsymbol{y}}$$

$$\min \frac{1}{2}\sum_{j=1}^{N}\sum_{i=1}^{N} s_{ij}(y_i - y_j)^2 = \min \mathbf{y}^T(\boldsymbol{D} - \mathbf{S})\mathbf{y}$$

Formulating the problem

$\min_{\mathbf{y}} \mathbf{y}^T(\boldsymbol{D}-\mathbf{S})\mathbf{y}$

- Has a trivial solution with $\boldsymbol{y} = \mathbf{0}$
- We need to constraint the solution and potentially regularize
- Let's have a look at $\boldsymbol{D}$



$$\boldsymbol{D} \quad \begin{array}{c|ccccc} & \boldsymbol{x}_1 & \boldsymbol{x}_2 & \boldsymbol{x}_3 & \boldsymbol{x}_4 & \boldsymbol{x}_5 \\ \hline \boldsymbol{x}_1 & 3 & 0 & 0 & 0 & 0 \\ \boldsymbol{x}_2 & 0 & 2 & 0 & 0 & 0 \\ \boldsymbol{x}_3 & 0 & 0 & 3 & 0 & 0 \\ \boldsymbol{x}_4 & 0 & 0 & 0 & 2 & 0 \\ \boldsymbol{x}_5 & 0 & 0 & 0 & 0 & 2 \end{array}$$

Laplacian eigenmaps

Matrix **D** provides a natural measure on the data points. The bigger the value d_{ii} (corresponding to point *i*) is, the more "important" the point *i* is

Let's make all points y "equally" important in the latent space

$$\min \mathbf{y}^T(\mathbf{D}-\boldsymbol{S})\mathbf{y} \ \text{ s.t. } \boldsymbol{y}^T\mathbf{D}\mathbf{y}=1$$

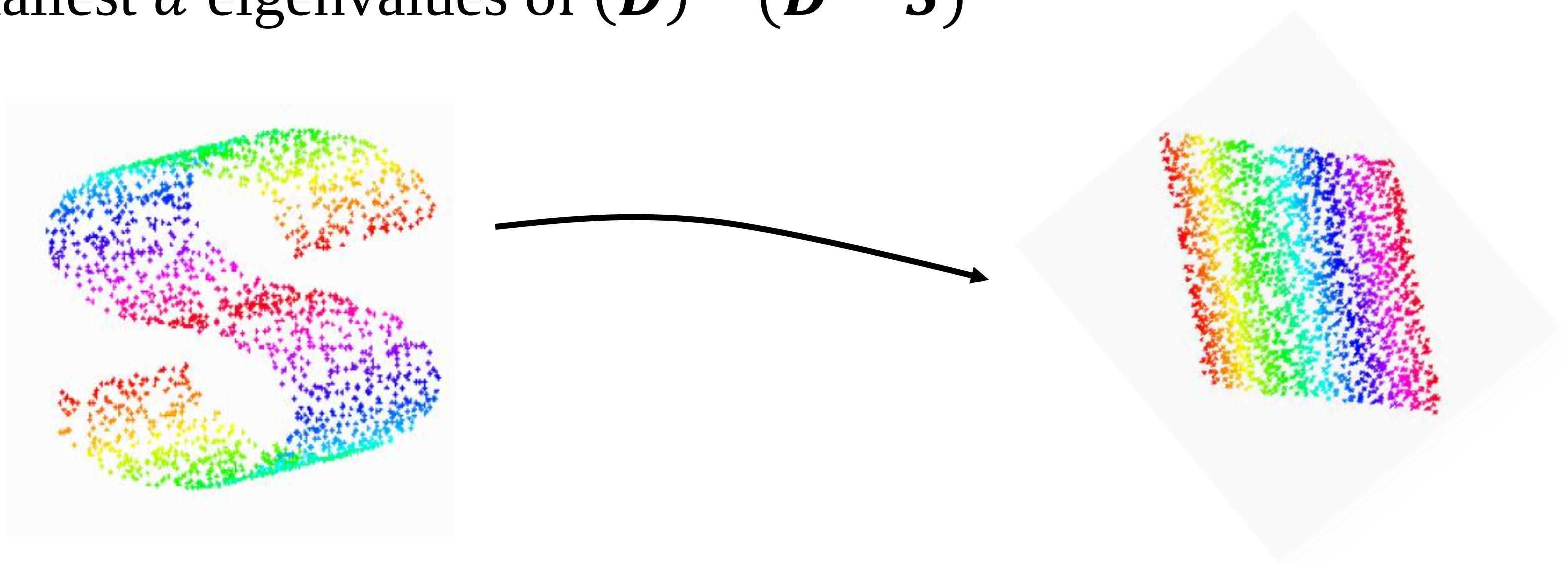
$$\mathbf{y} \text{ is the smallest (non} - \text{zero)eigenvector of } (\boldsymbol{D})^{-1}(\boldsymbol{D}-\boldsymbol{S})$$

Laplacian eigenmaps

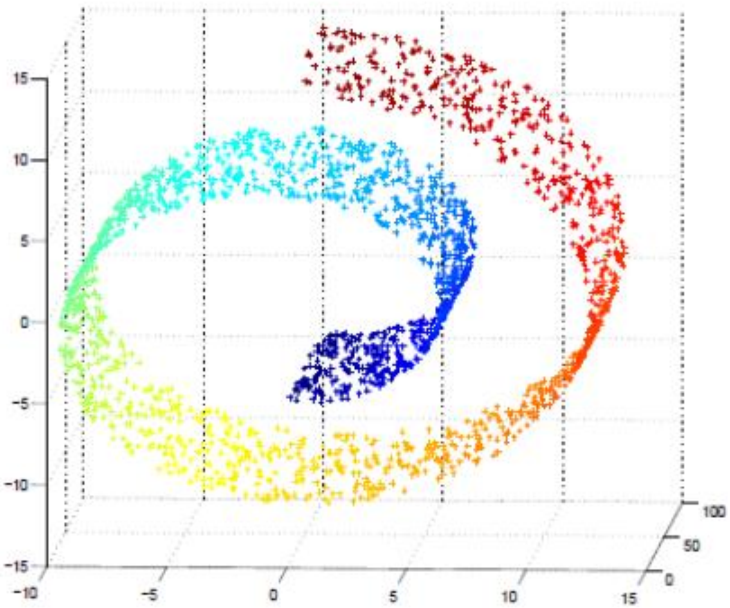
If we want more dimensions?

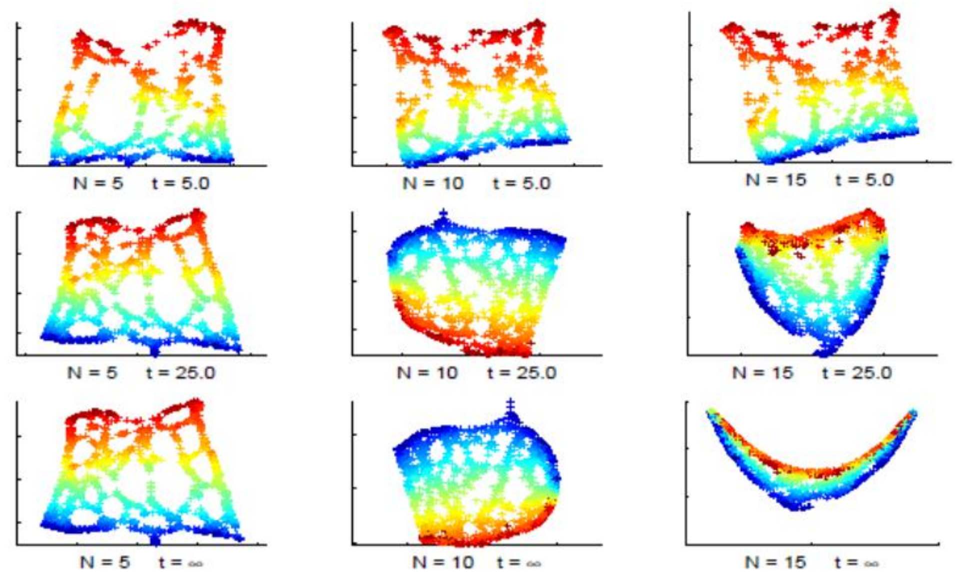
$$\min \operatorname{tr}[\boldsymbol{Y}(\boldsymbol{D}-\boldsymbol{S})\boldsymbol{Y}^{\boldsymbol{T}}] \text{ s.t. } \boldsymbol{Y}\boldsymbol{D}\boldsymbol{Y}^{\boldsymbol{T}} = \boldsymbol{I}$$

$\boldsymbol{Y}$ has as rows the (non − zero) eigenvectors that correspond to smallest d eigenvalues of $(\boldsymbol{D})^{-1}(\boldsymbol{D}-\boldsymbol{S})$



Laplacian eigenmaps





N number of neighbours and *t* the variance of the heat kernel

Locality preserving projections

The method is non-linear (why)?

It is quite difficult to embed new points in the latent space

$$\boldsymbol{y}_i = \boldsymbol{W}^T \boldsymbol{x}_i \qquad \boldsymbol{Y} = \boldsymbol{W}^T \boldsymbol{X}$$

$$\min \operatorname{tr}[\boldsymbol{Y}(\boldsymbol{D} - \boldsymbol{S})\boldsymbol{Y}^{\boldsymbol{T}}] \text{ s.t. } \boldsymbol{Y}\boldsymbol{D}\boldsymbol{Y}^{\boldsymbol{T}} = \boldsymbol{I}$$

$$\xRightarrow[\boldsymbol{Y}=\boldsymbol{W}^T\boldsymbol{X}]{} \min \operatorname{tr}[\boldsymbol{W}^T\boldsymbol{X}(\boldsymbol{D} - \boldsymbol{S})\boldsymbol{X}^{\boldsymbol{T}}\boldsymbol{W}] \text{ s.t. } \boldsymbol{W}^T\mathbf{X}\boldsymbol{D}\boldsymbol{X}^{\boldsymbol{T}}\boldsymbol{W} = \boldsymbol{I}$$

$\boldsymbol{W}$ has as colums the eigenvectors that correspond to smallest d eigenvalues of $[\boldsymbol{X}(\boldsymbol{D})\boldsymbol{X}^{\boldsymbol{T}}]^{-1}\boldsymbol{X}(\boldsymbol{D} - \boldsymbol{S})\boldsymbol{X}^{\boldsymbol{T}}$

Lecture summary

We studied three component analysis algorithms

PCA: Preserves global structure

LDA: Preserves/enhances class structure

LPP: Preserves/enhances local structure