Spectral Clustering

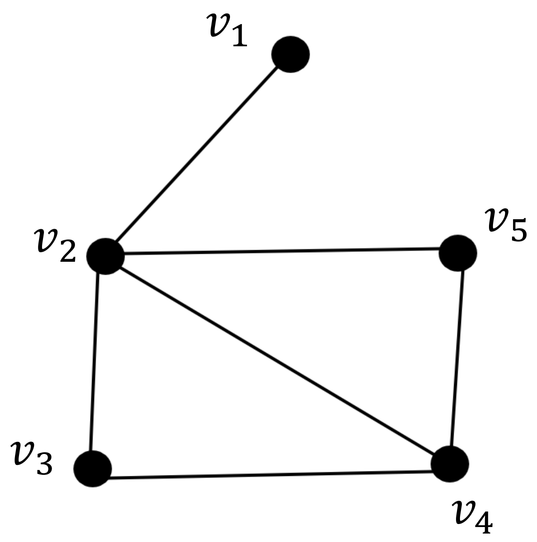
Mustafa Hajij

Graph Laplacian

Let G be a graph on n nodes. The Graph Laplacian is an n by n matrix given by :

$$L = D - A$$

Where D is the degree matrix and A is the adjacency matrix



$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \end{bmatrix} \quad D = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{bmatrix} \quad L = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 4 & -1 & -1 & -1 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & -1 & -1 & 3 & -1 \\ 0 & -1 & 0 & -1 & 2 \end{bmatrix}$$

Symmetric Graph Laplacian

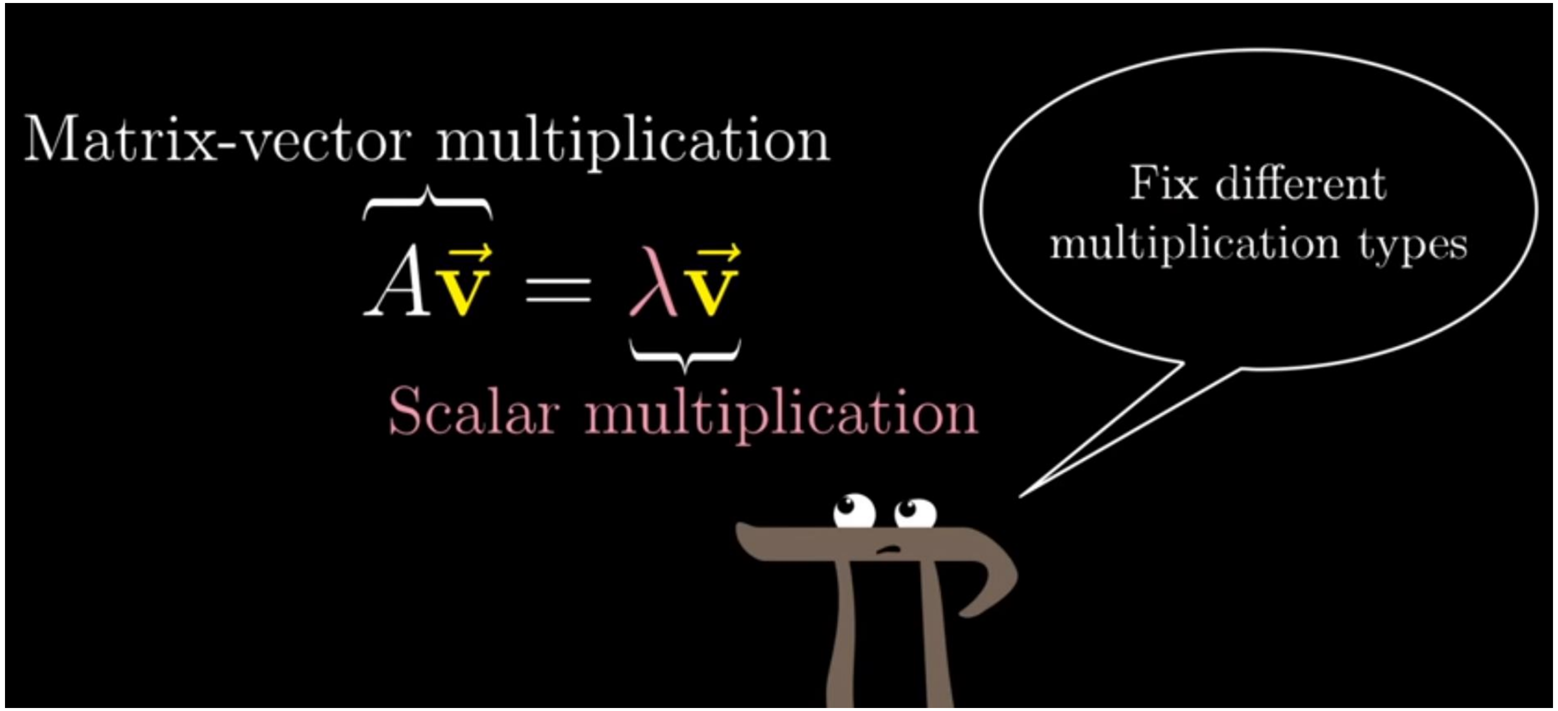
$$L^{\text{sym}} := D^{-1/2} L D^{-1/2} = I - D^{-1/2} A D^{-1/2},$$

Explicitly this is given by:

$$L^{\text{sym}}_{i,j} := \begin{cases} 1 & \text{if } i = j \text{ and } \deg(v_i) \neq 0 \\ -\frac{1}{\sqrt{\deg(v_i)\deg(v_j)}} & \text{if } i \neq j \text{ and } v_i \text{ is adjacent to } v_j \\ 0 & \text{otherwise.} \end{cases}$$

Eigenvalues and Eignenvector of a matrix

Watch this lecture for a review of the concepts of the eigenvalues and eigenvectors



Eigenvalues and Eignenvector of a symmetric matrix

A squared matrix is symmetric if $A = A^T$

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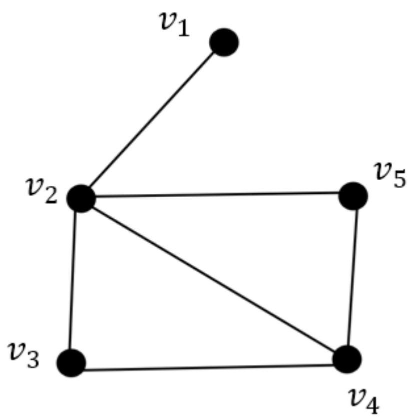

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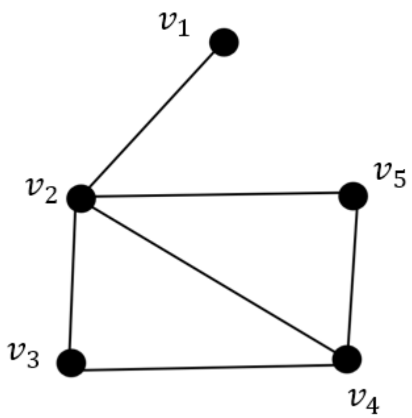

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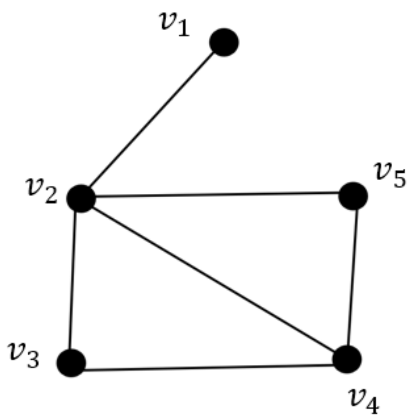

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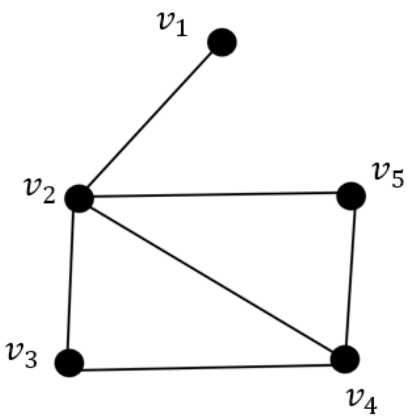

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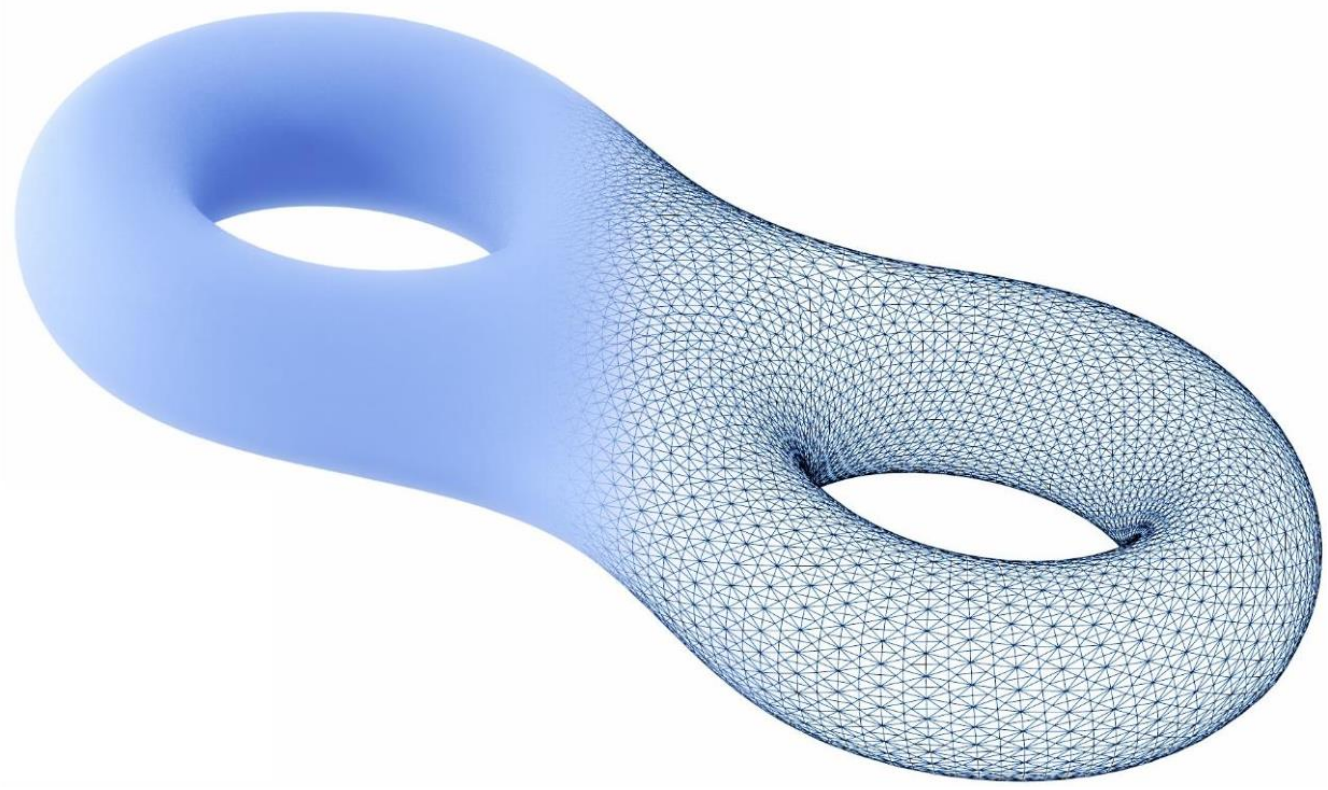
Solve its eigenvalues →

All of them are going to be real and non-negative

Eigenvalues and Eignenvector of the Laplacian

We can think about a mesh as a graph. We can compute the eigenvalues
And eigenvectors of the Laplacian of this graph



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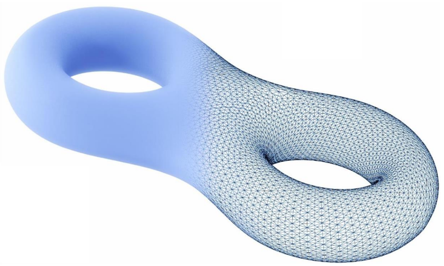


The first 10 eigenvectors of this mesh

Eigenvalues and Eignenvector in Python

In python you can compute the eigenvalues and the eigenvectors of a matrix : numpy.linalg.eig

From the data to the graph

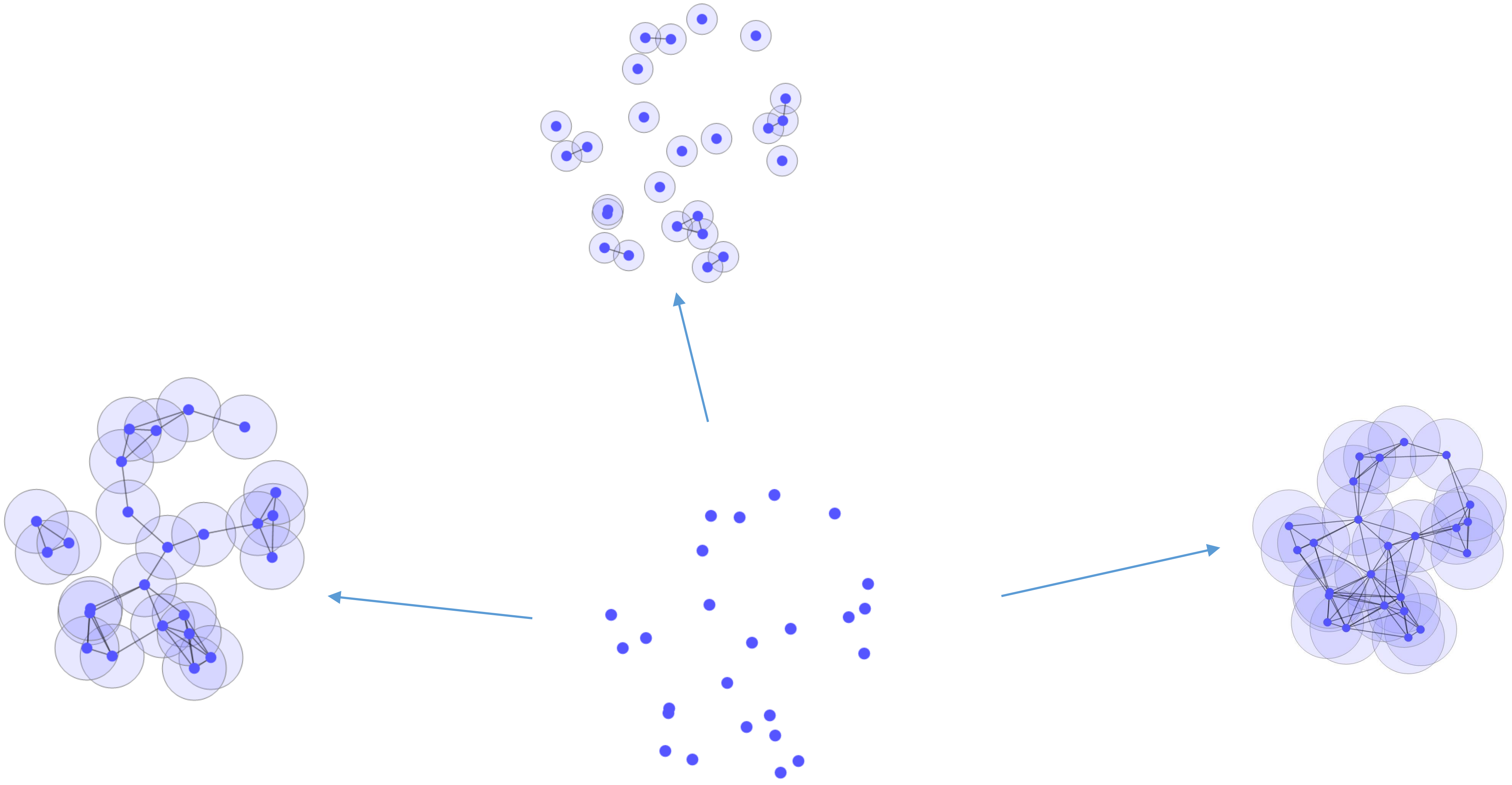
Given the data $X = \{p_1, p_2, \ldots, p_n\}$, we begin by constructing a graph G on the top of the data X:

- The points in X are the vertices of the graph
- The edges in the graph and their weights are determined by how close together and are in X

Three common methods to construct graphs :

- The neighborhood graphs ($\varepsilon -$ neighborhood graph or the knn graph)
- The complete graph on the set X.

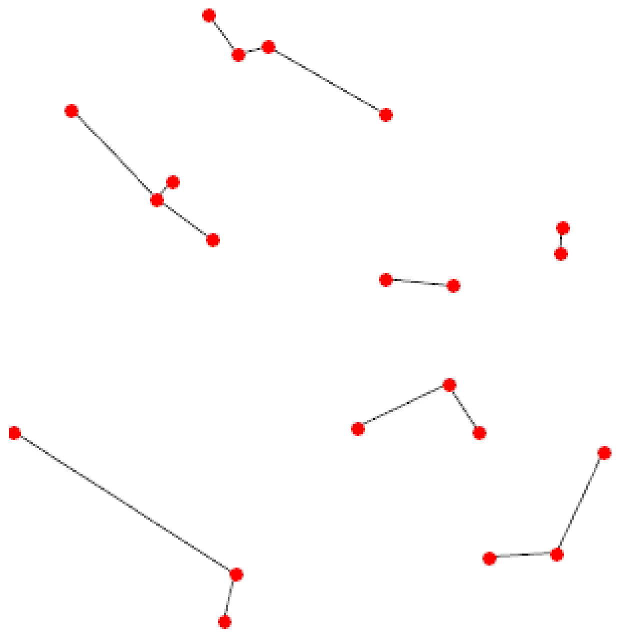
Similarity Graph:ε- Neighborhood Graph



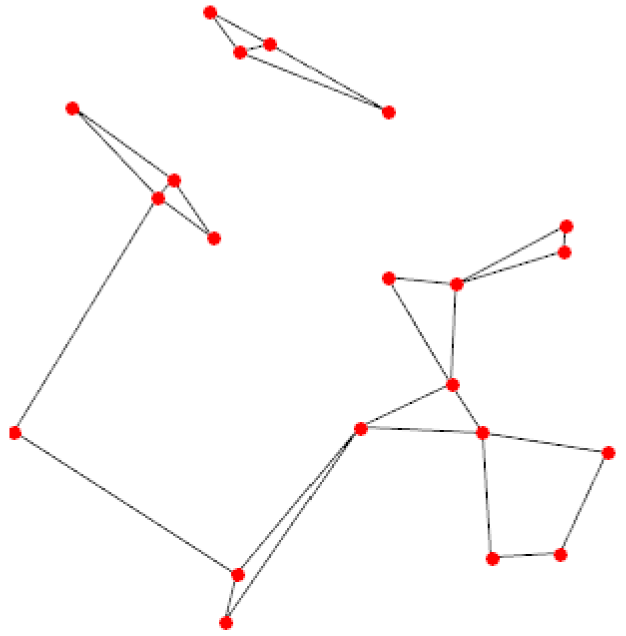
$$Construct\ the\ \varepsilon - neighborhood\ graph$$

A common problem here is which ε we should choose?

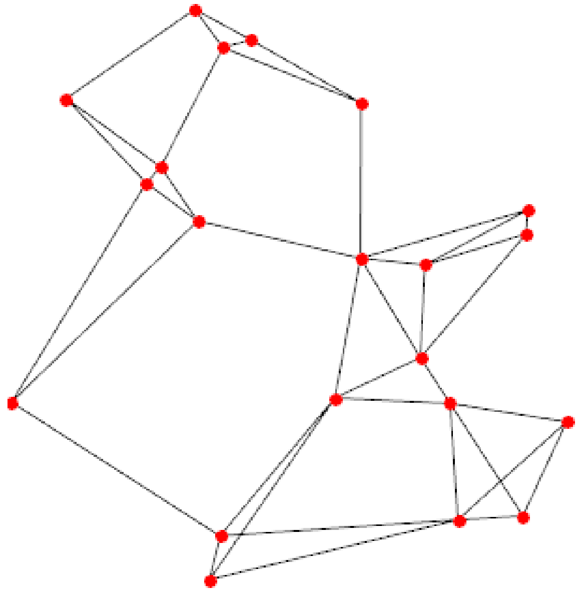
Similarity Graph: KNN Graph



Example of 1-NN graph



Example of 2-NN graph



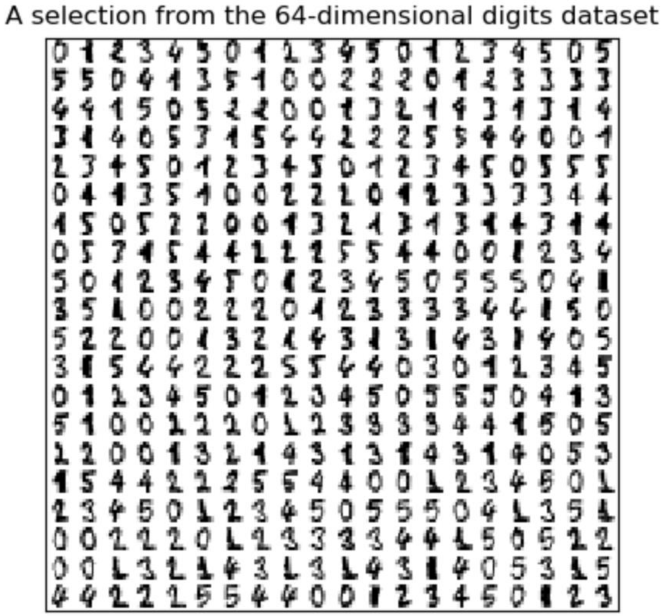
Example of 3-NN graph

Similarity Graph: The fully connected graph

Suppose that we are given a set of points $X = \{p_1, p_2, \dots, p_n\}$ in R^d. Another way to construct a graph on the top of the data X is by connecting all points in X to each other. In this case we weight all edges by $s_{ij} := s(x_i, x_j)$ defined as follows :

$$s(x_i, x_j) = \exp(-\frac{\|x_i - x_j\|^2}{2\sigma^2})$$

Spectral Embedding :example



spectral embedding

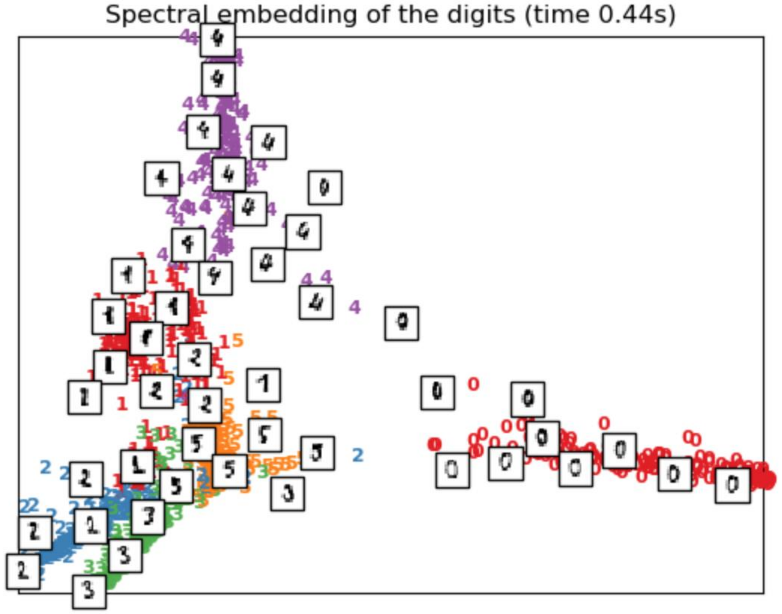


Image source: sklearn example

- The spectral embedding can unfold the nonlinear structures in a data in a high-dimensional feature space so that they become much easier to handle and understand.

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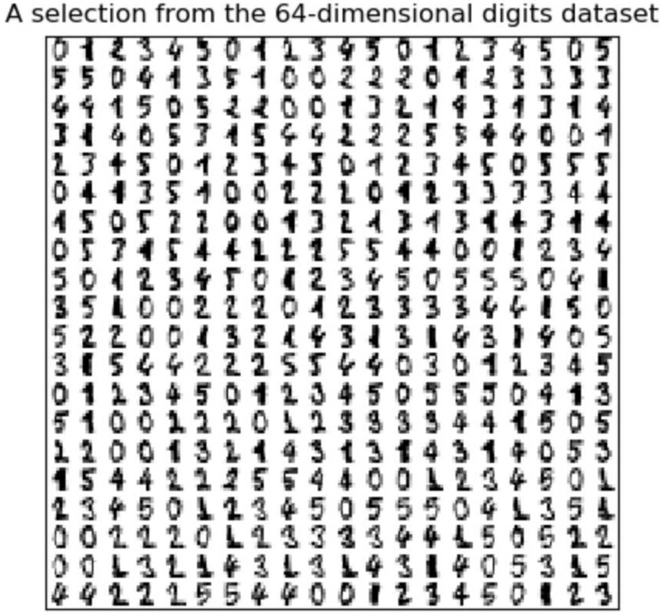

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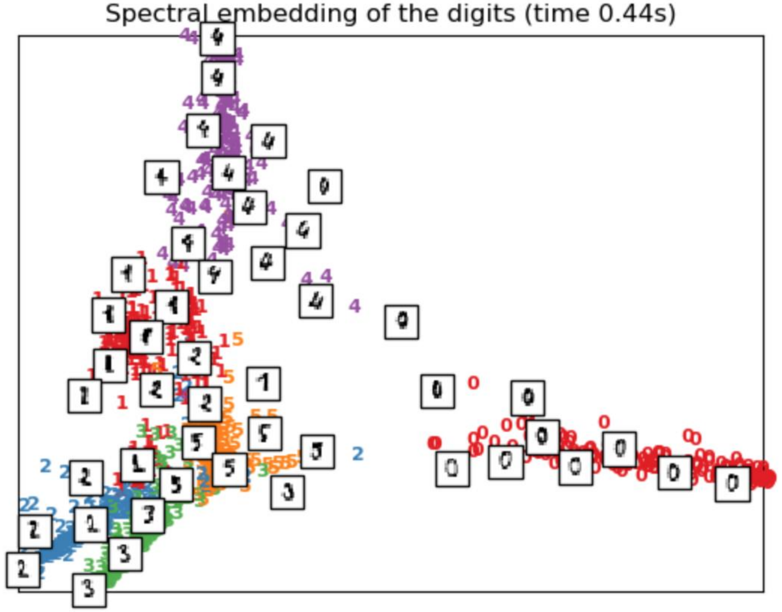

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$x = [x_1, \ldots, x_{64}]$

$w = [w_1, w_2]$

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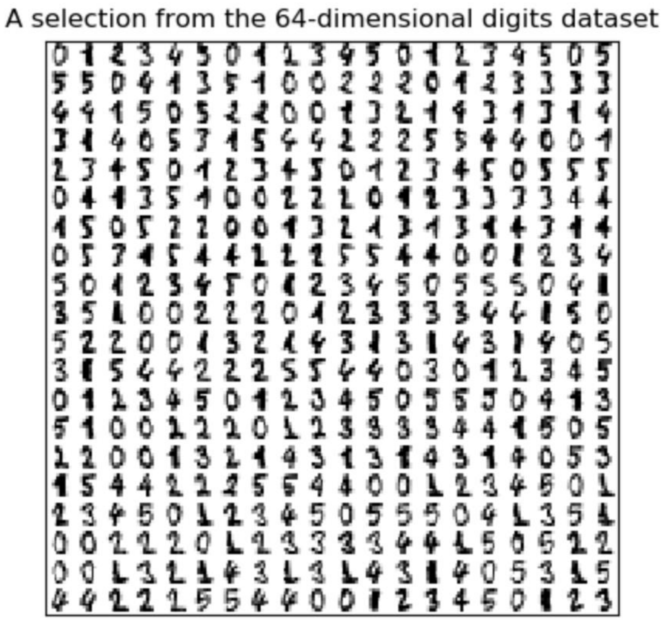

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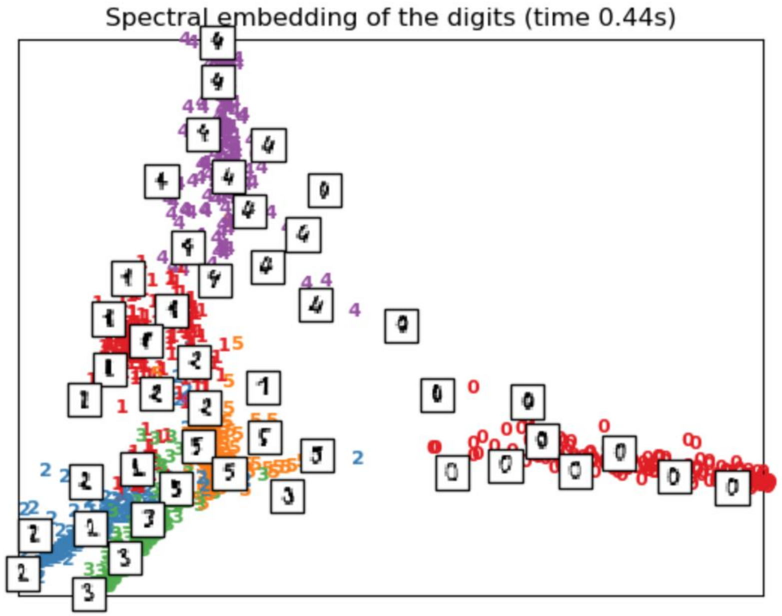

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$x = [x_1, \dots, x_{64}]$ spectral embedding $w = [w_1, w_2]$

Consider the digit dataset. This dataset can be thought of as a high-dimensional data with $d = 64$.

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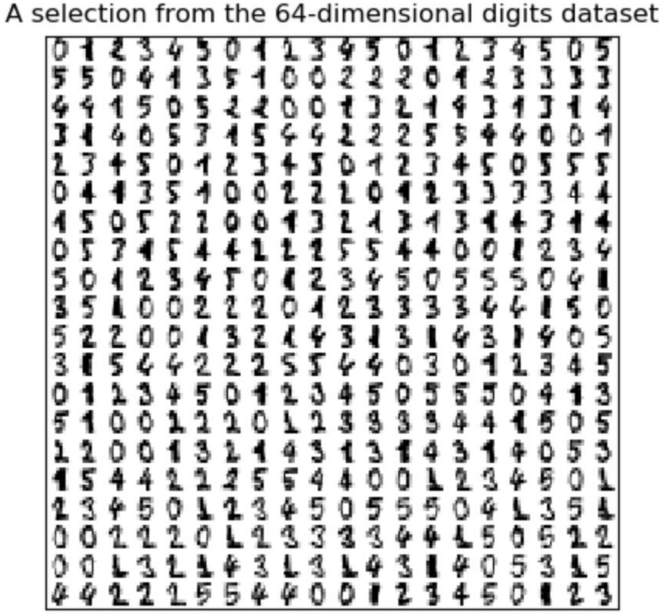

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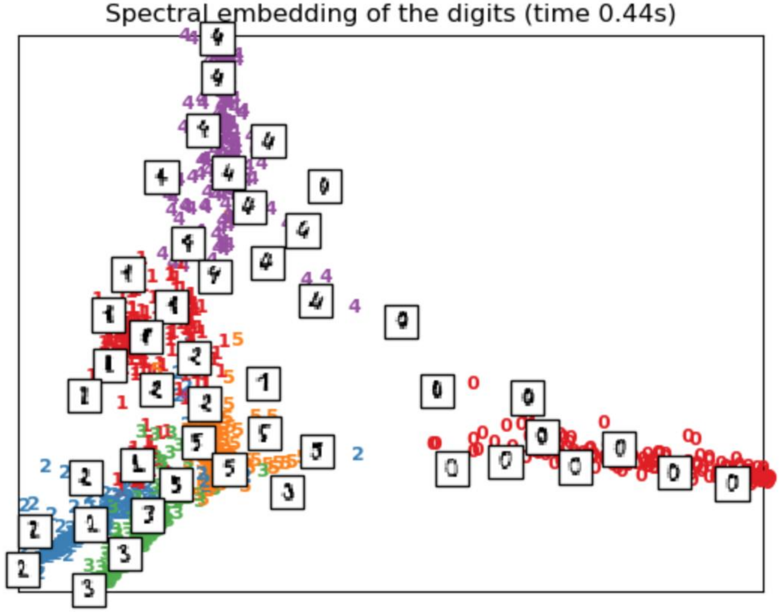

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$x = [x_1, \dots, x_{64}]$ — spectral embedding → $w = [w_1, w_2]$

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So every image can be thought of as a vector $x = [x_1, \dots, x_{64}]$

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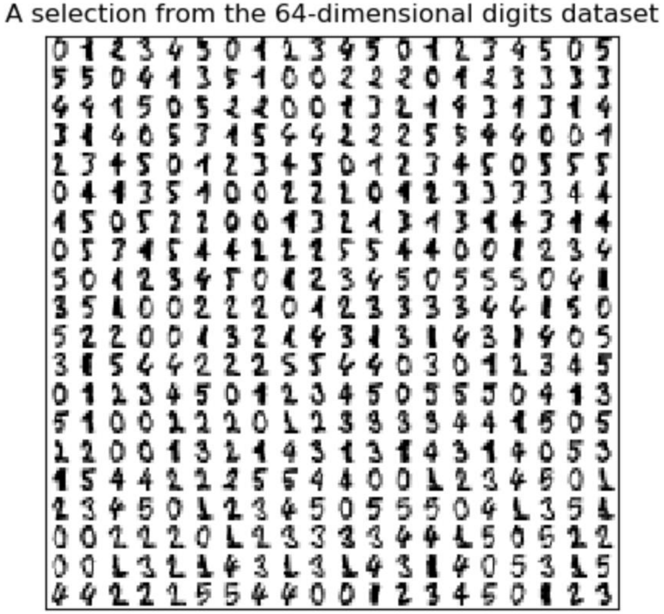

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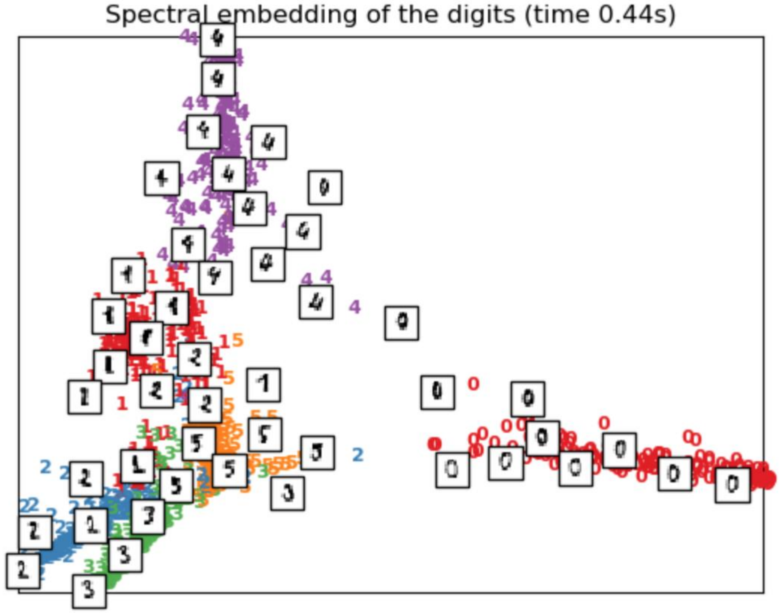

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Spectral embedding assigns to the point x new coordinates $w = [w_1, \ldots, w_k]$ where $k \leq 64$. Usually we choose $d << k$. In the example above we choose $k = 2$.

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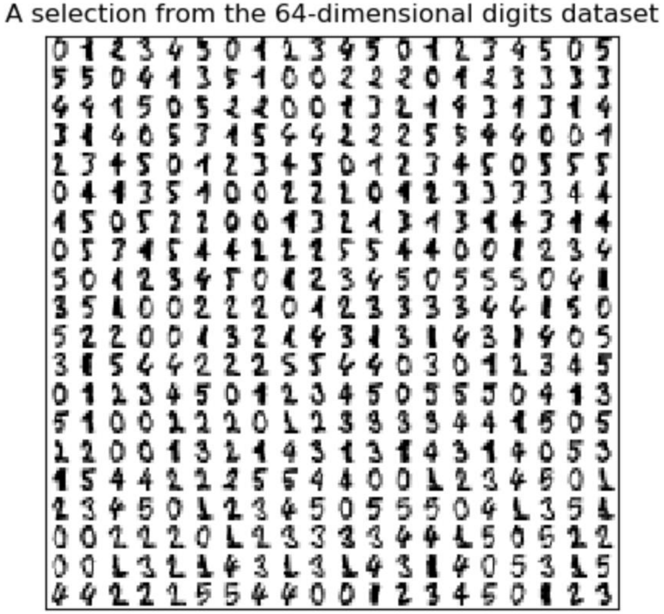

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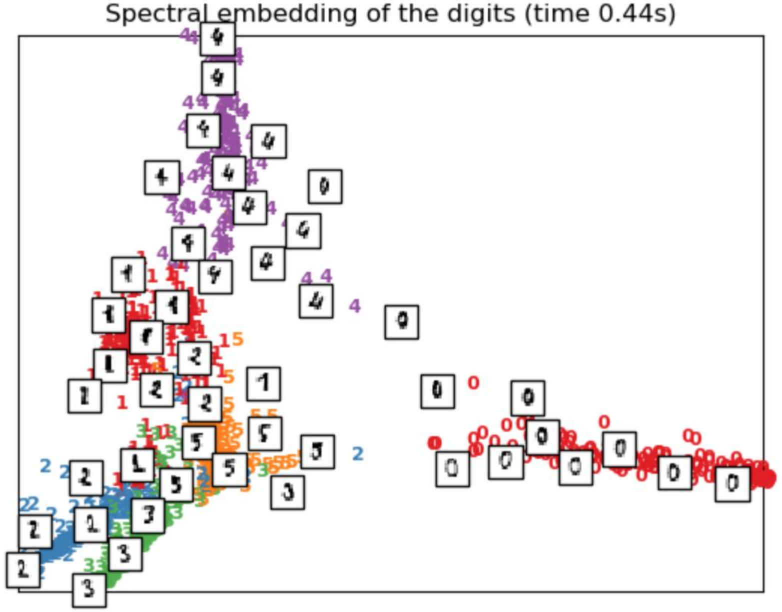

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But how exactly do we construct this new vector w ?

Spectral Embedding : general steps

- Construct a similarity graph phase : A similarity graph for the data X is chosen from the many available neighborhood graphs we studied in earlier lectures.

- The spectral embedding phase :In this step we use the eigenvectors of the Laplacian of the similarity graph to construct new coordinates.

Spectral Embedding : Algorithm

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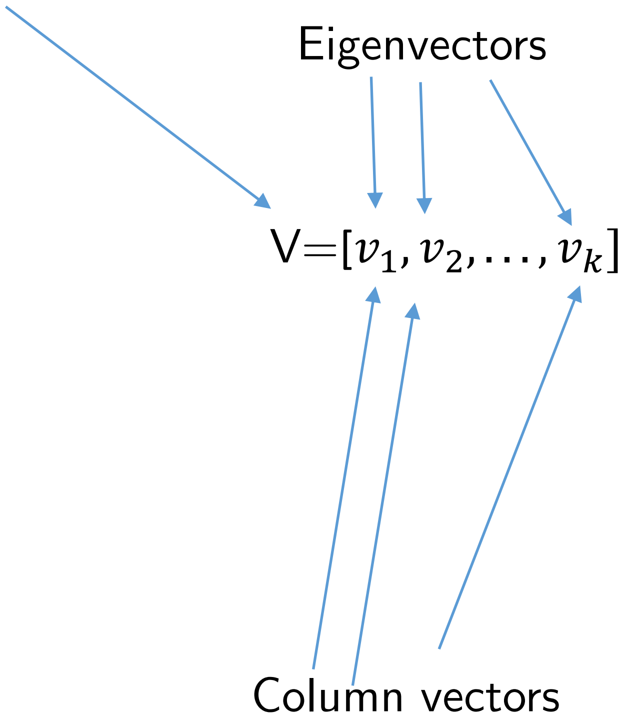

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- Form W from V by normalizing the rows of W (making every row a unit vector).

Eigenvectors

$$V=[v_1, v_2, \ldots, v_k]$$

Column vectors

$$v_{ij} = \frac{u_{ij}}{\left(\sum_{l=1}^{k} u_{il}^2\right)^2}$$

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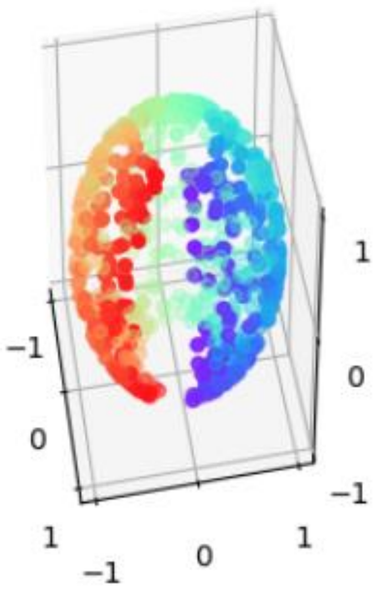
- Each row w_i in the matrix W is, by definition, the spectral embedding of the point x_i from the original data

Spectral Embedding :more examples



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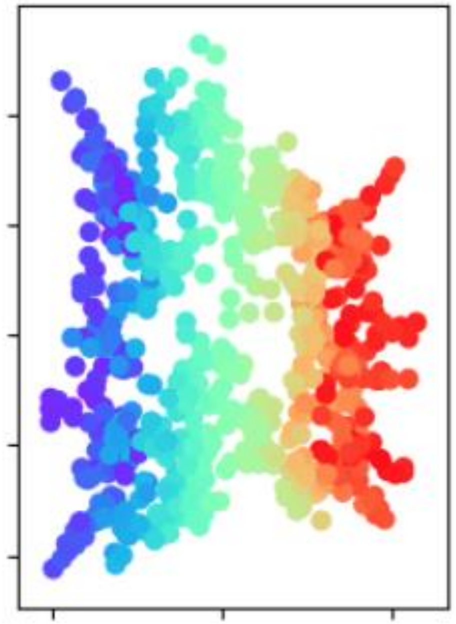

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Image source: sklearn example

In general the results of spectral embedding can better reveal or exaggerate useful underlying structures in the input data.

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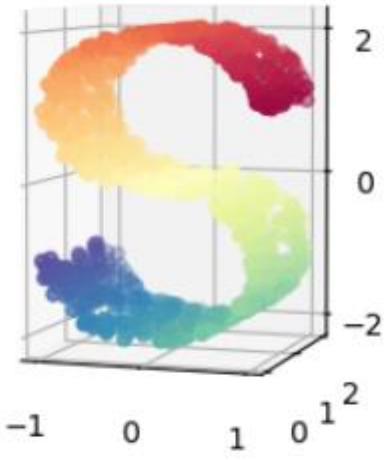

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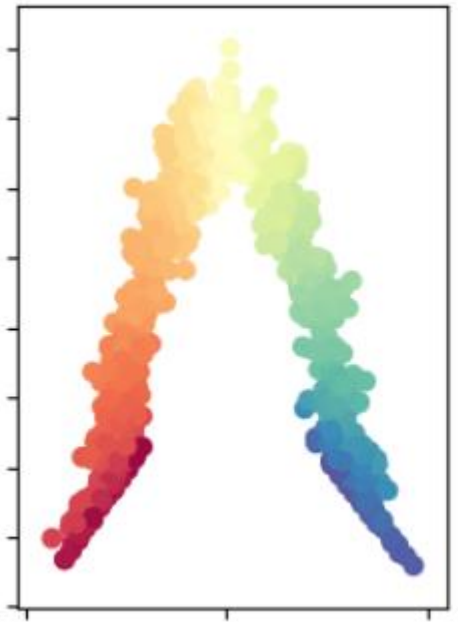

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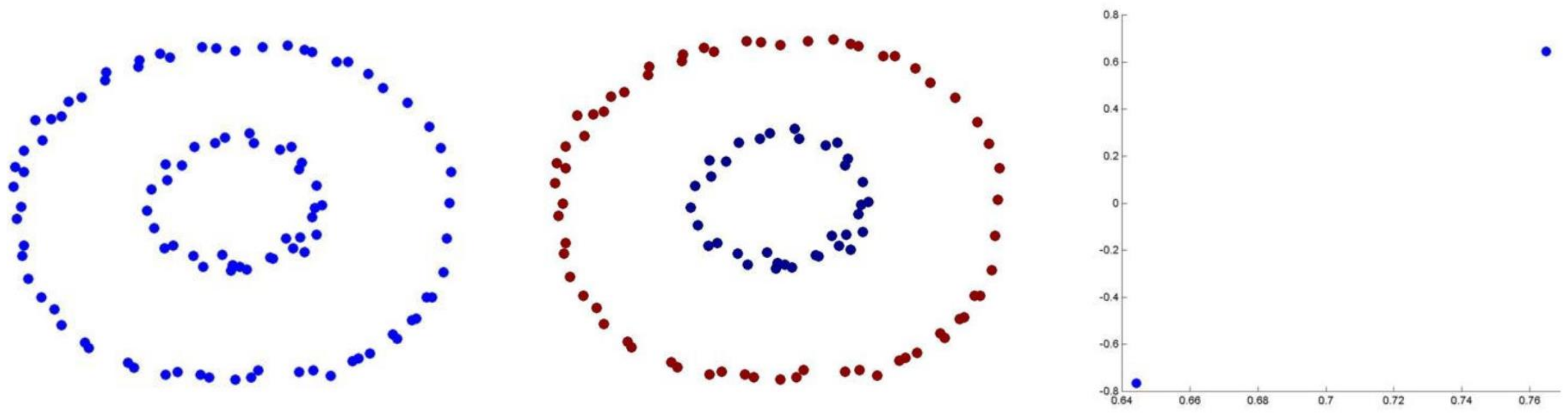

(a) (b) (c) Image [source]()

- In the above example the dataset (a) is mapped to its clustering embedding (figure c) which can be trivially classified using k-means (figure c).
- This example shows that via by a transforming the data into the spectral domain, certain intrinsic shape structures are revealed.

Spectral Clustering : general steps

- Construct a similarity graph phase : A similarity graph for the data X is chosen among the many available neighborhood graphs we studied in earlier lectures.

- The spectral embedding phase :In this step we use the eigenvectors of the Laplacian of the similarity graph to construct new coordinates for the points in X in which the clusters are more obvious.

- Using one of the classical clustering algorithms to cluster the points in the spectral space and induce this clustering results to the original points.

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- x_i is assigned to cluster α iff row i of W is assigned to cluster α.

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- Construct a similarity graph G=G(X) of the data. This can be the k-NN graph for instance.
- Compute the Laplacian of the graph L(G).
- Compute top k eigenvectors of L and place them as columns in a matrix V
- Form W from V by normalizing the rows of W (making every row a unit vector).

(Spectral embedding)

- Run K-means to cluster the row vectors of W
- x_i is assigned to cluster α iff row i of W is assigned to cluster α.

More Spectral Clustering: examples

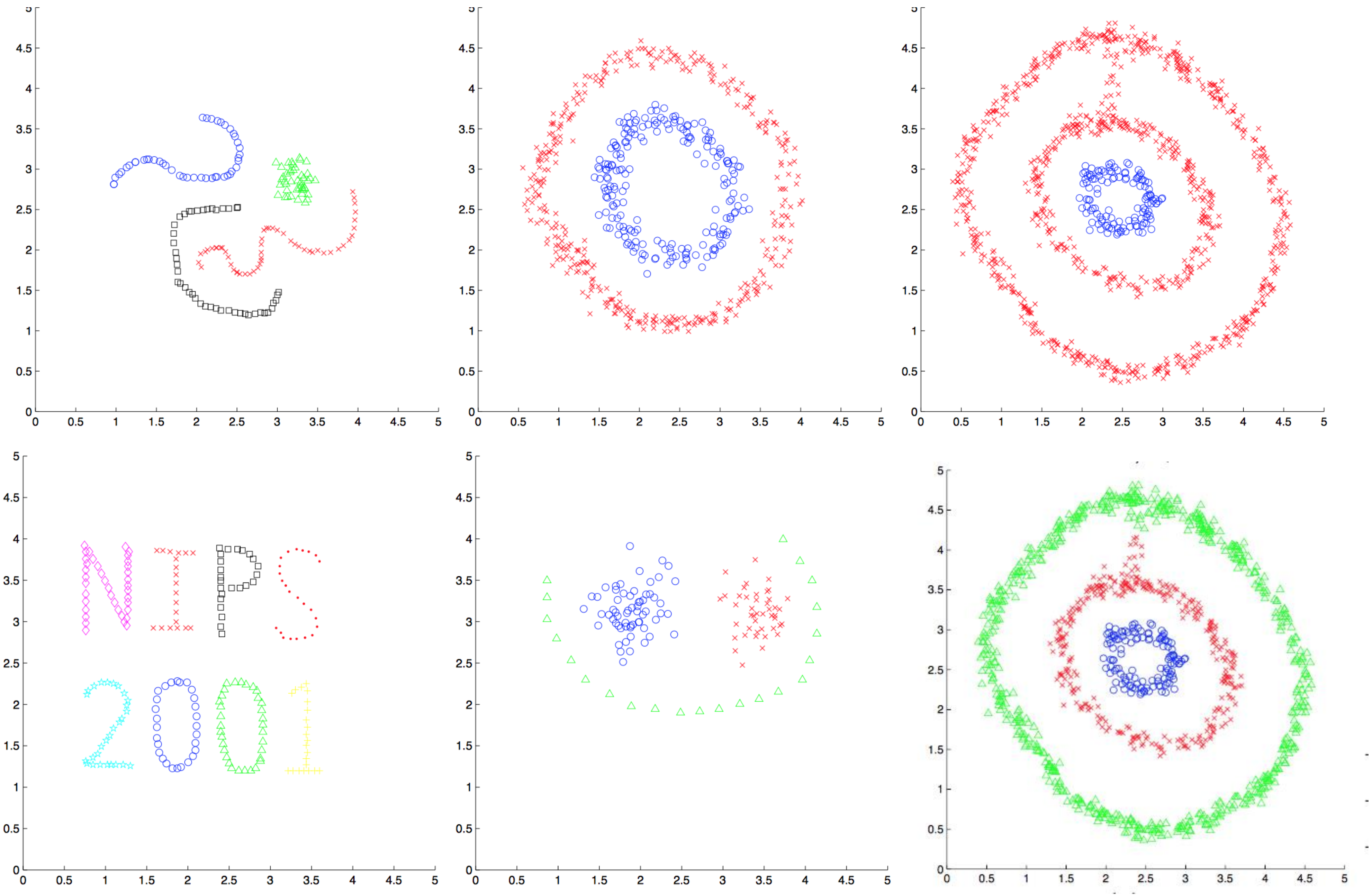
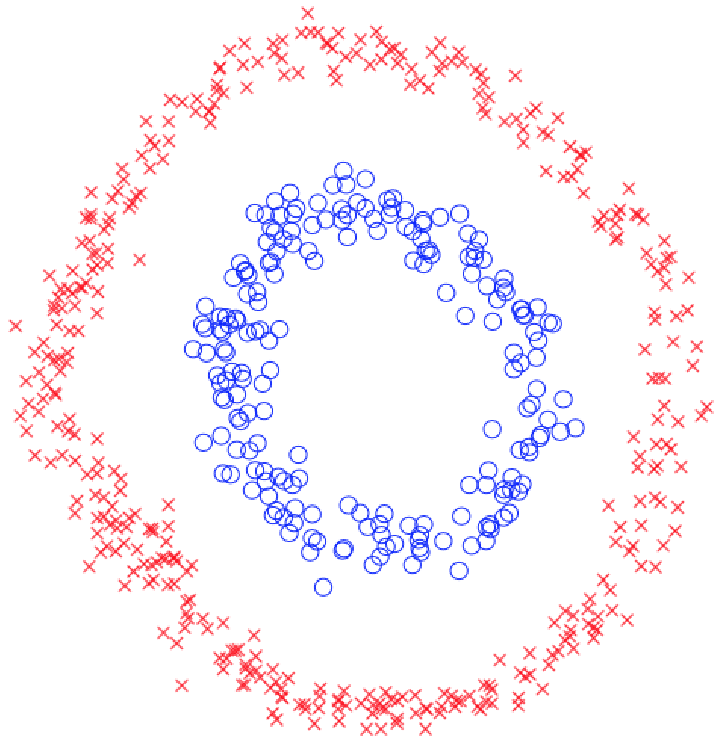
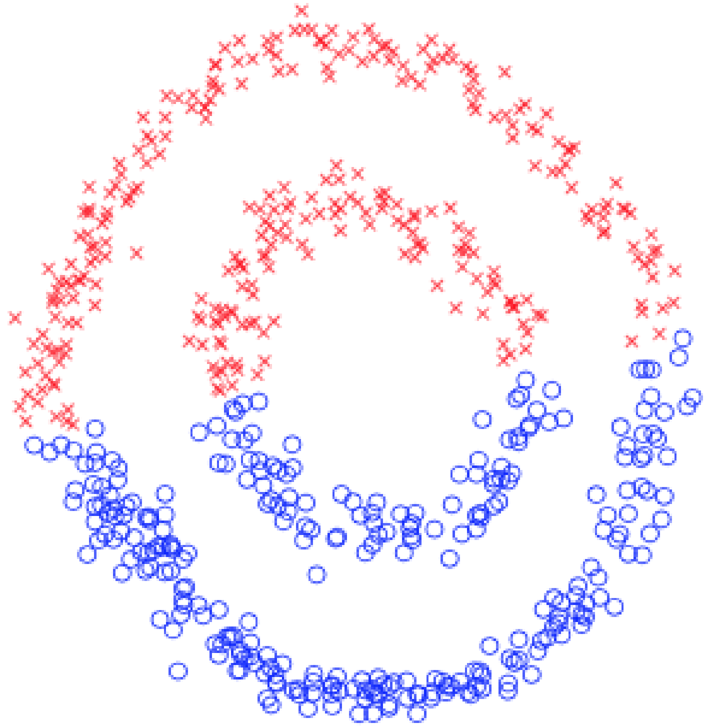


image source

Spectral Clustering vs K-means



Spectral clustering

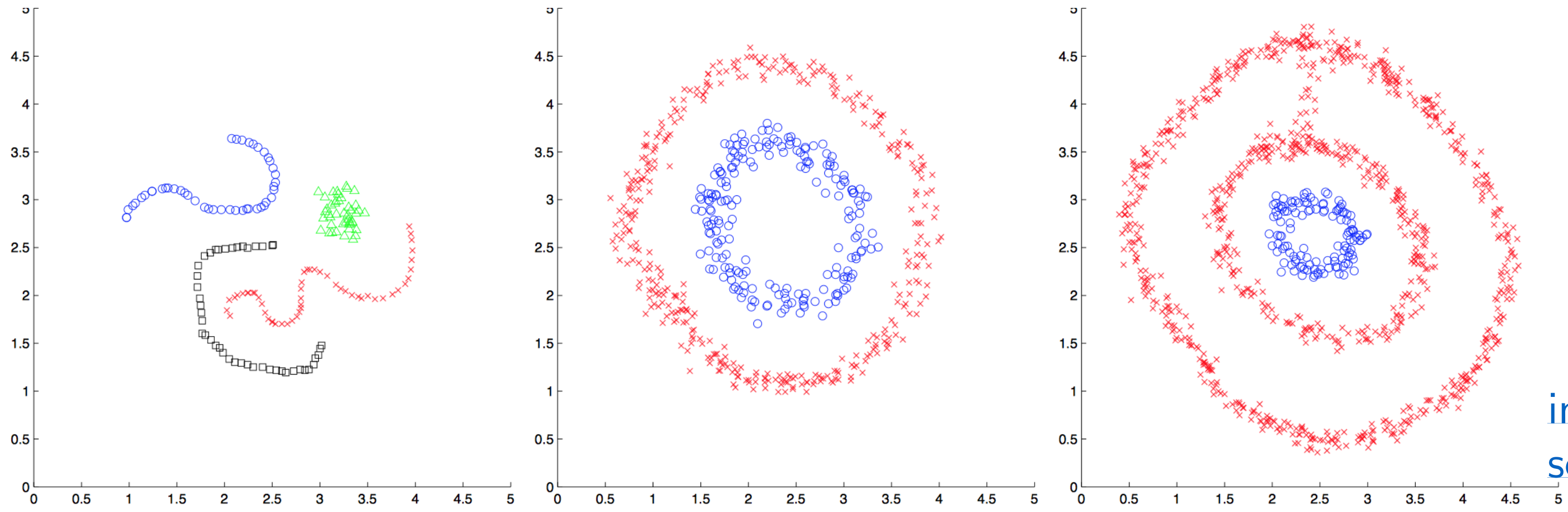


K-means clustering

image source

Spectral Clustering/Embedding: remarks

Spectral clustering does not put any assumption on the shape of data.



[image source](#)

Spectral clustering can be used to for clustering non-linearly separable data.

The results of spectral embedding can better reveal or exaggerate useful underlying structures in the input data.