

# PA 2018 - 06

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## Spectral Clustering:

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### Step 0:

Given a set of points  $S = s_1, s_2, \dots, s_n$  in  $R^l$

### Step 1:

Compute affinities  $A \in R^{n \times n}$ ,  $A_{ij} = e^{\frac{-||s_i - s_j||_2^2}{2\sigma^2}}$ ,  $A_{ij} = 0$

### Step 2:

Let  $D = \text{diag}(\sum_j A_{1j}, \sum_j A_{2j}, \dots, \sum_j A_{nj})$  of the row affinities, and set  $L = D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$

### Step 3:

Compute eigen decomposition of  $L$ .

Let  $X = (x_1, x_2, \dots, x_k)$ ,  $X \in R^{n \times k}$  denote a matrix consisting of the  $k$  "largest eigenvectors"  $x_1, \dots, x_k$  of  $L$

$k$  eigen vectors associated with the largest eigenvalues

### Step 4:

Normalize  $X$  :  $Y_{ij} = \frac{X_{ij}}{(\sum_j X_{ij}^2)^{\frac{1}{2}}}$

### Step 5:

Perform k-means clustering with  $k$  centers on the points that are the rows of  $Y$

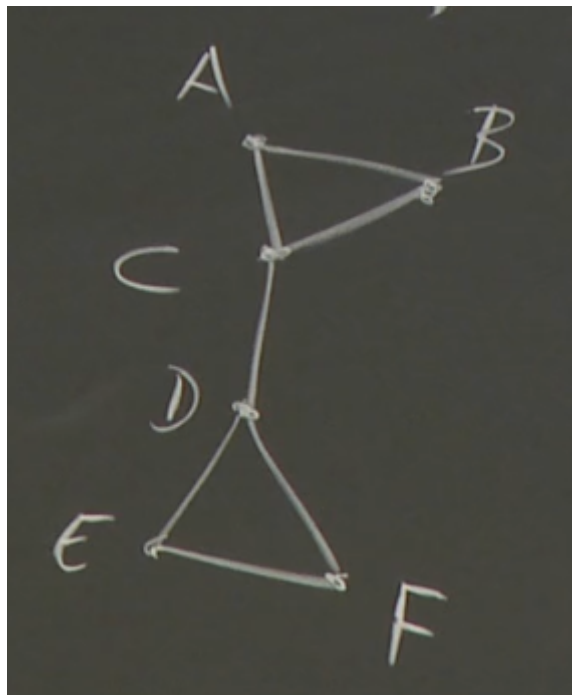
### Step 6:

The points in the original space are assigned to the  $k$  clusters of their transformed version in %Y%.

## Quick, informal note on the Graph Laplacian:

A tool that links graph theory linear algorithm and probability theory.

Let`s look for example at a graph.



Popular graph algorithm:

Maximum Flow between two nodes?

Shortest Path between two nodes?

The set of mathematical tools that can be used on a graph is somewhat limited, what exactly should we calculate on a list of nodes and edges?

⇒ Spectral Graph Theory opens a door to linear algebra by treating a graph's adjacency matrix as an actual matrix in an algebraic sense ⇒ we can for example compute the eigenvalues to find out invariants about the underlying graph.

**adjacency matrix:** A useful representation of the adjacency matrix is the Graph Laplacian  $L$ .

## Remarks on the "Ideal Case" (Sec. 3. 1)

- The set of eigenvalues of a block matrix  $\hat{L} = \begin{bmatrix} L^{(11)} & 0 & 0 \\ 0 & L^{(22)} & 0 \\ 0 & 0 & L^{(33)} \end{bmatrix}$  is identical to the set of  $\text{eigenvalue}(L^{(11)})$ ,  $\text{eigenvalue}(L^{(22)})$ ,  $\text{eigenvalue}(L^{(33)})$  (can be treated independently)
- The largest eigenvalue of a graph Laplacian is 1, the second largest is lower than 1 ⇒  $\hat{L}$  has exactly 3 eigenvalues that are 1. These are the 3 largest ones that we are looking for.
- The associated 3 eigenvectors are orthogonal and thus span a 3-dimensional subspace. Not, however, that the exact choice of eigenvectors is not unique.

The points are clustering around the rotation axes span the subspace. These axes are spanned by  $90^\circ$  angles between them. Therefore, k-means can easily cluster the point in that subspace.

## Sec. 3.2 clusters that lie close to another:

The distribution of eigenvalues indicates how well the data structure fits into  $k$  clusters: consider the eigenvalue gap  $\sigma = |\lambda_k - \lambda_{k+1}|$

**Cheeger constant:**

$$h(S_i) = min_I \frac{\sum_{j \in I, k \notin I} A_{jk}}{min\{\sum_{j \in I} d_j^{(i)}, \sum_{k \notin I} d_k^{(i)}\}}$$

$$\left[\begin{array}{ccc} L^{(11)} & 0 & 0 \\ 0 & L^{(22)} & 0 \\ 0 & 0 & L^{(33)} \end{array}\right]$$