Data Analysis and Manifold Learning
Lecture 7: Spectral Clustering

Radu Horaud
INRIA Grenoble Rhone-Alpes, France
Radu.Horaud@inrialpes.fr
http://perception.inrialpes.fr/

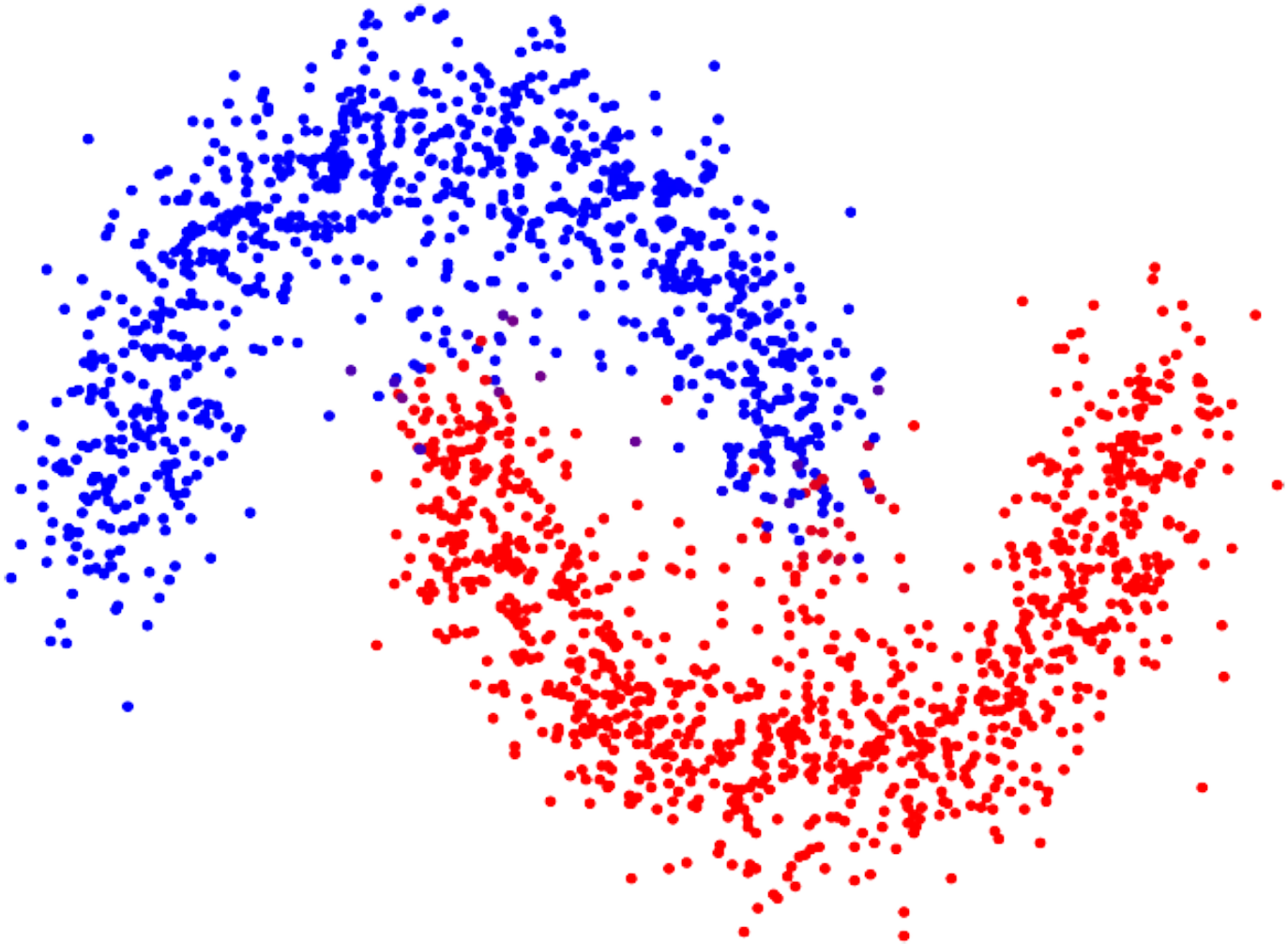
Outline of Lecture 7

- What is spectral clustering?
- We will use the material of Lecture 3
- We will discuss several spectral clustering algorithms
- Link between spectral clustering and graph partitioning
- Lind between spectral clustering and random walks on graphs

Material for this lecture

- F. R. K. Chung. Spectral Graph Theory. 1997. (Chapter 1)
- M. Belkin and P. Niyogi. Laplacian Eigenmaps for Dimensionality Reduction and Data Representation. Neural Computation, 15, 1373–1396 (2003).
- U. von Luxburg. A Tutorial on Spectral Clustering. Statistics and Computing, 17(4), 395–416 (2007). (An excellent paper)
- Software: `http://open-specmatch.gforge.inria.fr/index.php`. Computes, among others, Laplacian embeddings of very large graphs.

Example

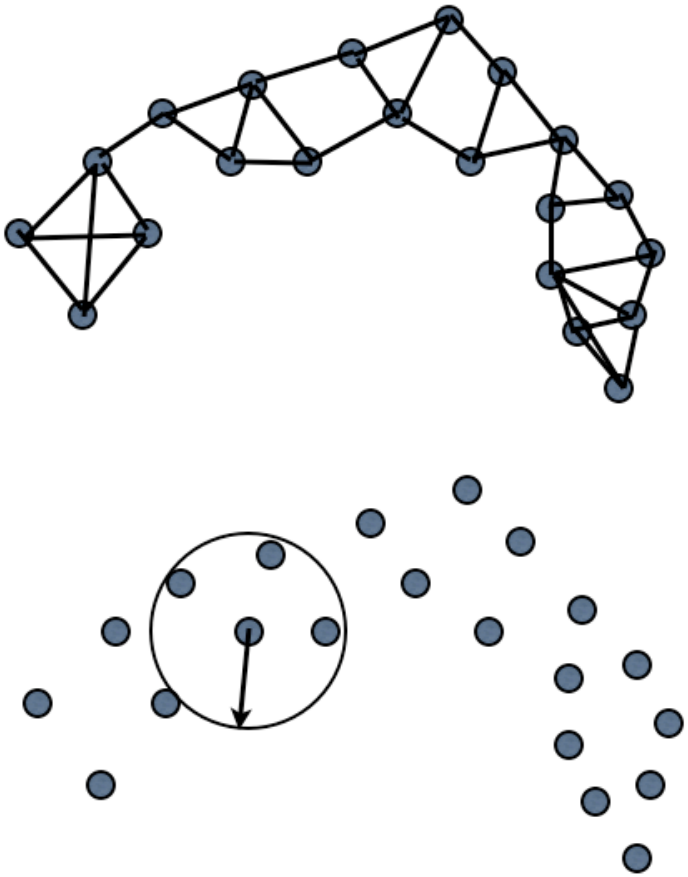


Which Clustering Method to Use?

- Techniques such as K-means or Gaussian mixtures will not work well because the clusters are neither spherical nor Gaussian.
- One needs to apply a non-linear transformation of the data such that "curved" clusters are transformed into "blobs"
- The general idea of spectral clustering is to build an undirected weigthed graph and to map the points (the graph's vertices) into the *spectral* space, spanned by the eigenvectors of the Laplacian matrix.

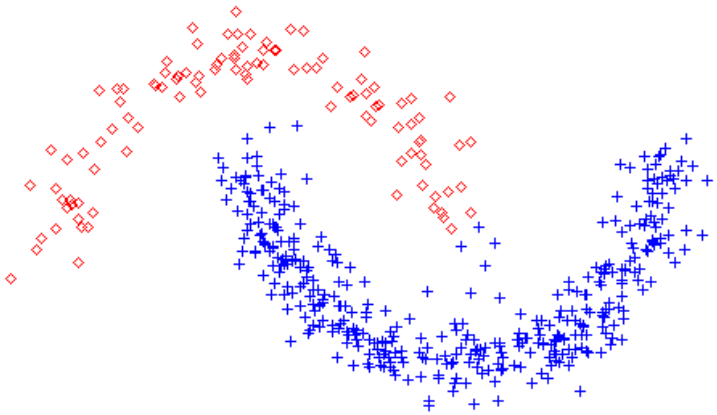
Building a Graph from a Point Cloud

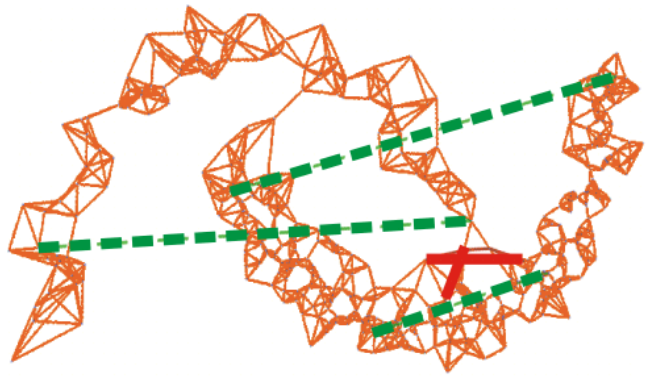
- K-nearest neighbor (KNN) rule
- ε-radius rule
- Other more sophisticated rules can be found in the literature, i.e., Lee and Verleysen. Nonlinear Dimensionality Reduction (Appendix E). Springer. 2007.



- Graph building is still an active research topic.

An Example of Graph Building





The Graph Partitioning Problem

- We want to find a partition of the graph such that the edges between different groups have very low weight, while the edges within a group have high weight.
- **The mincut problem**:
  1. Edges between groups have very low weight, and
  2. Edges within a group have high weight.
  3. Choose a partition of the graph into k groups that mimimizes the following criterion:

$$\text{mincut}(A_1, \ldots, A_k) := \frac{1}{2} \sum_{i=1}^{k} W(A_i, \overline{A}_i)$$

- with

$$W(A, B) = \sum_{i \in A, j \in B} w_{ij}$$

RatioCut and NormalizedCut

- Often, the mincut solution isolates a vertex from the rest of the graph.
- Request that the groups are reasonably large.
- **Ratio cut** (Hagen & Kahng 1992) minimizes:

$$\text{RatioCut}(A_1, \ldots, A_k) := \frac{1}{2} \sum_{i=1}^{k} \frac{W(A_i, \overline{A}_i)}{|A_i|}$$

- Here $|A|$ refers to the number of vertices in group A.
- **Normalized cut**: (Shi & Malik 2000)

$$\text{NCut}(A_1, \ldots, A_k) := \frac{1}{2} \sum_{i=1}^{k} \frac{W(A_i, \overline{A}_i)}{\text{vol}(A_i)}$$

What is Spectral Clustering?

- Both ratio-cut and normalized-cut minimizations are NP-hard problems
- Spectral clustering is a way to solve relaxed versions of these problems:
  1. The smallest non-null eigenvectors of the *unnormalized Laplacian* approximate the RatioCut minimization criterion, and
  2. The smallest non-null eigenvectors of the *random-walk Laplacian* approximate the NormalizedCut criterion.

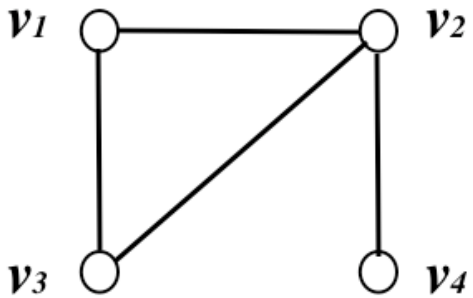
The Laplacian matrix of a graph

- $f : \mathcal{V} \longrightarrow \mathbb{R}$, i.e., $f(v_1), \ldots, f(v_n)$.
- $(\mathbf{L}\boldsymbol{f})(v_i) = \sum_{v_j \sim v_i} (f(v_i) - f(v_j))$
- Connection between the Laplacian and the adjacency matrices:

$$\mathbf{L} = \mathbf{D} - \mathbf{A}$$

- The degree matrix: $\mathbf{D} := D_{ii} = d(v_i)$.

$$\mathbf{L} = \begin{bmatrix} 2 & -1 & -1 & 0 \\ -1 & 3 & -1 & -1 \\ -1 & -1 & 2 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix}$$



Matrices of an undirected weighted graph

- We consider *undirected weighted graphs*; Each edge e_{ij} is weighted by $w_{ij} > 0$. We obtain:

$$\mathbf{\Omega} := \begin{cases} \Omega_{ij} = w_{ij} & \text{if there is an edge } e_{ij} \\ \Omega_{ij} = 0 & \text{if there is no edge} \\ \Omega_{ii} = 0 \end{cases}$$

- The degree matrix: $\mathbf{D} = \sum_{i \sim j} w_{ij}$

The Laplacian on an undirected weighted graph

- $\mathbf{L} = \mathbf{D} - \mathbf{\Omega}$
- The Laplacian as an operator:

$$(\mathbf{L}\boldsymbol{f})(v_i) = \sum_{v_j \sim v_i} w_{ij}(f(v_i) - f(v_j))$$

- As a quadratic form:

$$\boldsymbol{f}^\top \mathbf{L} \boldsymbol{f} = \frac{1}{2} \sum_{e_{ij}} w_{ij}(f(v_i) - f(v_j))^2$$

- $\mathbf{L}$ is symmetric and positive semi-definite $\leftrightarrow$ $w_{ij} \geq 0$.
- $\mathbf{L}$ has n non-negative, real-valued eigenvalues: $0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$.

The Laplacian in Practice

- A graph vertex v_i is associated with a point $\boldsymbol{x}_i \in \mathbb{R}^D$.
- The weight w_{ij} of an edge e_{ij} is defined by the Gaussian kernel:

$$w_{ij} = \exp\left(-\|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2/\sigma^2\right)$$

- This defines a similarity function between two *nearby* points.

Other adjacency matrices

- The *normalized weighted adjacency matrix*

$$\mathbf{\Omega}_N = \mathbf{D}^{-1/2}\mathbf{\Omega}\mathbf{D}^{-1/2}$$

- The *transition* matrix of the Markov process associated with the graph:

$$\mathbf{\Omega}_R = \mathbf{D}^{-1}\mathbf{\Omega} = \mathbf{D}^{-1/2}\mathbf{\Omega}_N\mathbf{D}^{1/2}$$

Several Laplacian matrices

- The *unnormalized Laplacian* which is also referred to as the *combinatorial Laplacian* $\mathbf{L}_C$,
- the *normalized Laplacian* $\mathbf{L}_N$, and
- the *random-walk Laplacian* $\mathbf{L}_R$ also referred to as the *discrete Laplace operator*.

We have:

$$\begin{aligned}
\mathbf{L}_C &= \mathbf{D} - \mathbf{\Omega} \\
\mathbf{L}_N &= \mathbf{D}^{-1/2}\mathbf{L}_C\mathbf{D}^{-1/2} = \mathbf{I} - \mathbf{\Omega}_N \\
\mathbf{L}_R &= \mathbf{D}^{-1}\mathbf{L}_C = \mathbf{I} - \mathbf{\Omega}_R
\end{aligned}$$

Some spectral properties of the Laplacians

Laplacian	Null space	Eigenvalues	Eigenvectors
$\mathbf{L}_C = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\top$	$\boldsymbol{u}_1 = \mathbf{1}$	$0 = \lambda_1 < \lambda_2 \leq \ldots \leq \lambda_n \leq 2\max_i(d_i)$	$\boldsymbol{u}_{i>1}^\top \mathbf{1} = 0$, $\boldsymbol{u}_i^\top \boldsymbol{u}_j = \delta_{ij}$
$\mathbf{L}_N = \mathbf{W}\mathbf{\Gamma}\mathbf{W}^\top$	$\boldsymbol{w}_1 = \mathbf{D}^{1/2}\mathbf{1}$	$0 = \gamma_1 < \gamma_2 \leq \ldots \leq \gamma_n \leq 2$	$\boldsymbol{w}_{i>1}^\top \mathbf{D}^{1/2}\mathbf{1} = 0$, $\boldsymbol{w}_i^\top \boldsymbol{w}_j = \delta_{ij}$
$\mathbf{L}_R = \mathbf{T}\mathbf{\Gamma}\mathbf{T}^{-1}$ $\mathbf{T} = \mathbf{D}^{-1/2}\mathbf{W}$	$\boldsymbol{t}_1 = \mathbf{1}$	$0 = \gamma_1 < \gamma_2 \leq \ldots \leq \gamma_n \leq 2$	$\boldsymbol{t}_{i>1}^\top \mathbf{D}\mathbf{1} = 0$, $\boldsymbol{t}_i^\top \mathbf{D}\boldsymbol{t}_j = \delta_{ij}$

Spectral properties of adjacency matrices

From the relationship between the normalized Laplacian and adjacency matrix: $\mathbf{L}_N = \mathbf{I} - \mathbf{\Omega}_N$ one can see that their eigenvalues satisfy $\gamma = 1 - \delta$.

Adjacency matrix	Eigenvalues	Eigenvectors
$\mathbf{\Omega}_N = \mathbf{W}\mathbf{\Delta}\mathbf{W}^\top$, $\mathbf{\Delta} = \mathbf{I} - \mathbf{\Gamma}$	$-1 \leq \delta_n \leq \ldots \leq \delta_2 < \delta_1 = 1$	$\boldsymbol{w}_i^\top \boldsymbol{w}_j = \delta_{ij}$
$\mathbf{\Omega}_R = \mathbf{T}\mathbf{\Delta}\mathbf{T}^{-1}$	$-1 \leq \delta_n \leq \ldots \leq \delta_2 < \delta_1 = 1$	$\boldsymbol{t}_i^\top \mathbf{D} \boldsymbol{t}_j = \delta_{ij}$

The Laplacian of a graph with one connected component

- $\mathbf{L}\boldsymbol{u} = \lambda \boldsymbol{u}$.
- $\mathbf{L}\mathbf{1} = \mathbf{0}$, $\lambda_1 = 0$ is the smallest eigenvalue.
- The *one* vector: $\mathbf{1} = (1 \dots 1)^\top$.
- $0 = \boldsymbol{u}^\top \mathbf{L} \boldsymbol{u} = \sum_{i,j=1}^{n} w_{ij}(u(v_i) - u(v_j))^2$.
- If any two vertices are connected by a path, then $\boldsymbol{u} = (u(v_1), \dots, u(v_n))$ needs to be constant at all vertices such that the quadratic form vanishes. Therefore, a graph with one connected component has the constant vector $\boldsymbol{u}_1 = \mathbf{1}$ as the only eigenvector with eigenvalue 0.

A graph with $k > 1$ connected components

- Each connected component has an associated Laplacian. Therefore, we can write matrix $\mathbf{L}$ as a *block diagonal matrix*:

$$\mathbf{L} = \begin{bmatrix} \mathbf{L}_1 & & \\ & \ddots & \\ & & \mathbf{L}_k \end{bmatrix}$$

- The spectrum of $\mathbf{L}$ is given by the union of the spectra of $\mathbf{L}_i$.
- Each block corresponds to a connected component, hence each matrix $\mathbf{L}_i$ has an eigenvalue 0 with multiplicity 1.
- The spectrum of $\mathbf{L}$ is given by the union of the spectra of $\mathbf{L}_i$.
- The eigenvalue $\lambda_1 = 0$ has multiplicity k.

The eigenspace of $\lambda_1 = 0$ with multiplicity k

- The eigenspace corresponding to $\lambda_1 = \ldots = \lambda_k = 0$ is spanned by the k mutually orthogonal vectors:

$$\begin{aligned} \boldsymbol{u}_1 &= \mathbf{1}_{L_1} \\ &\ldots \\ \boldsymbol{u}_k &= \mathbf{1}_{L_k} \end{aligned}$$

- with $\mathbf{1}_{L_i} = (0000111110000)^\top \in \mathbb{R}^n$
- These vectors are the *indicator vectors* of the graph's connected components.
- Notice that $\mathbf{1}_{L_1} + \ldots + \mathbf{1}_{L_k} = \mathbf{1}$

The Fiedler vector of the graph Laplacian

- The first non-null eigenvalue λ_{k+1} is called the Fiedler value.
- The corresponding eigenvector $\boldsymbol{u}_{k+1}$ is called the Fiedler vector.
- The multiplicity of the Fiedler eigenvalue depends on the graph's structure and it is difficult to analyse.
- The Fiedler value is the *algebraic connectivity of a graph*, the further from 0, the more connected.
- The Fiedler vector has been extensively used for *spectral bi-partioning*
- Theoretical results are summarized in Spielman & Teng 2007: `http://cs-www.cs.yale.edu/homes/spielman/`

Eigenvectors of the Laplacian of connected graphs

- $\boldsymbol{u}_1 = \mathbf{1}, \mathbf{L}\mathbf{1} = \mathbf{0}$.
- $\boldsymbol{u}_2$ is the *the Fiedler vector* generally assumed with multiplicity 1.
- The eigenvectors form an orthonormal basis: $\boldsymbol{u}_i^\top \boldsymbol{u}_j = \delta_{ij}$.
- For any eigenvector $\boldsymbol{u}_i = (\boldsymbol{u}_i(v_1) \dots \boldsymbol{u}_i(v_n))^\top$, $2 \leq i \leq n$:

$$\boldsymbol{u}_i^\top \mathbf{1} = 0$$

- Hence the components of $\boldsymbol{u}_i$, $2 \leq i \leq n$ satisfy:

$$\sum_{j=1}^{n} \boldsymbol{u}_i(v_j) = 0$$

- Each component is bounded by:

$$-1 < \boldsymbol{u}_i(v_j) < 1$$

Spectral embedding using the *unnormalized* Laplacian

- Compute the eigendecomposition $\mathbf{L}_C = \mathbf{D} - \mathbf{\Omega} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\top$.
- Select the k smallest non-null eigenvalues $\lambda_2 \leq \ldots \leq \lambda_{k+1}$
- $\lambda_{k+2} - \lambda_{k+1} =$ **eigengap**.
- We obtain the $n \times k$ column-orthogonal matrix $\widetilde{\mathbf{U}} = [\boldsymbol{u}_2 \ldots \boldsymbol{u}_{k+1}]$:

$$\widetilde{\mathbf{U}} = \begin{bmatrix} \boldsymbol{u}_2(v_1) & \ldots & \boldsymbol{u}_{k+1}(v_1) \\ \vdots & & \vdots \\ \boldsymbol{u}_2(v_n) & \ldots & \boldsymbol{u}_{k+1}(v_n) \end{bmatrix}$$

- Embedding: The i-row of this matrix correspond to the representation of vertex v_I in the $\mathbb{R}^k$ basis spanned by the orthonormal vector basis $\boldsymbol{u}_2, \ldots, \boldsymbol{u}_{k+1}$.
- Therefore: $\mathbf{Y} = [\boldsymbol{y}_1 \ldots \boldsymbol{y}_i \ldots \boldsymbol{y}_n] = \widetilde{\mathbf{U}}^\top$

Spectral embedding using the random-walk Laplacian

- The $n \times k$ matrix contains the first k eigenvectors of $\mathbf{L}_R$:

$$\widetilde{\mathbf{W}} = \begin{bmatrix} \boldsymbol{w}_2 & \dots & \boldsymbol{w}_{k+1} \end{bmatrix}$$

- It is straightforward to obtain the following expressions, where $\boldsymbol{d}$ and $\mathbf{D}$ are the degree-vector and the degree-matrix:

$$\boldsymbol{w}_i^\top \boldsymbol{d} = 0, \ \forall i, 2 \leq i \leq n$$

$$\widetilde{\mathbf{W}}^\top \mathbf{D} \widetilde{\mathbf{W}} = \mathbf{I}_k$$

- Hence, vectors $\boldsymbol{w}_2, \dots, \boldsymbol{w}_{k+1}$ do not form an orthonormal basis.
- The embedding using the random-walk Laplacian:

$$\mathbf{Y} = [\boldsymbol{y}_1 \dots \boldsymbol{y}_i \dots \boldsymbol{y}_n] = \widetilde{\mathbf{W}}^\top$$

Spectral clustering using the random-walk Laplacian

- For details see (von Luxburg '07)
- Input: Laplacian $\mathbf{L}_r$ and the number k of clusters to compute.
- Output: Cluster $C_1, \ldots, C_k$.

1. Compute $\mathbf{W}$ formed with the first k eigenvectors of the random-walk Laplacian.
2. Determine the spectral embedding $\mathbf{Y} = \mathbf{W}^\top$
3. Cluster the columns $\boldsymbol{y}_j, j = 1, \ldots, n$ into k clusters using the K-means algorithm.

K-means clustering

See Bishop'2006 (pages 424–428) for more details.

- What is a cluster: a group of points whose inter-point distance are small compared to distances to points outside the cluster.
- Cluster centers: $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_k$.
- Goal: find an assignment of points to clusters as well as a set of vectors $\boldsymbol{\mu}_i$.
- Notations: For each point $\boldsymbol{y}_j$ there is a *binary indicator variable* $r_{ji} \in \{0, 1\}$.
- Objective: minimize the following *distorsion measure*:

$$J = \sum_{j=1}^{n} \sum_{i=1}^{k} r_{ji} \|\boldsymbol{y}_j - \boldsymbol{\mu}_i\|^2$$

The K-means algorithm

1. Initialization: Choose initial values for $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_k$.
2. First step: Assign the j-th point to the closest cluster center:

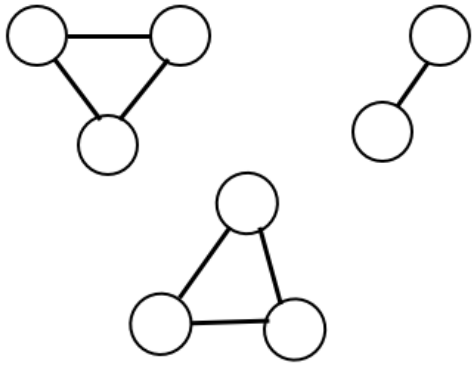
$$r_{ji} = \begin{cases} 1 & \text{if } i = \arg\min_l \|\boldsymbol{y}_j - \mu_l\|^2 \\ 0 & \text{otherwise} \end{cases}$$

3. Second Step: Minimize J to estimate the cluster centers:

$$\boldsymbol{\mu}_i = \frac{\sum_{j=1}^n r_{ji} \boldsymbol{y}_j}{\sum_{j=1}^n r_{ji}}$$

4. Convergence: Repeat until no more change in the assignments.

Spectral Clustering Analysis : The Ideal Case

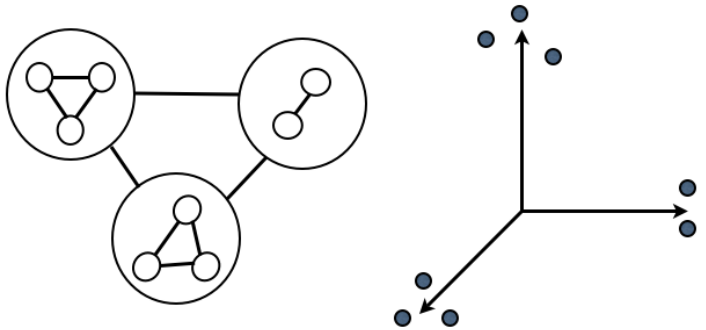


- $\lambda_1 = \lambda_2 = \lambda_3 = 0$
- $\boldsymbol{w}_1, \boldsymbol{w}_2, \boldsymbol{w}_3$ form an orthonormal basis.
- The connected components collapse to $(100), (010), (001)$.
- Clustering is trivial in this case.

$$\mathbf{W} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\mathbf{Y} = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix}$$

Spectral Clustering Analysis : The Perturbed Case



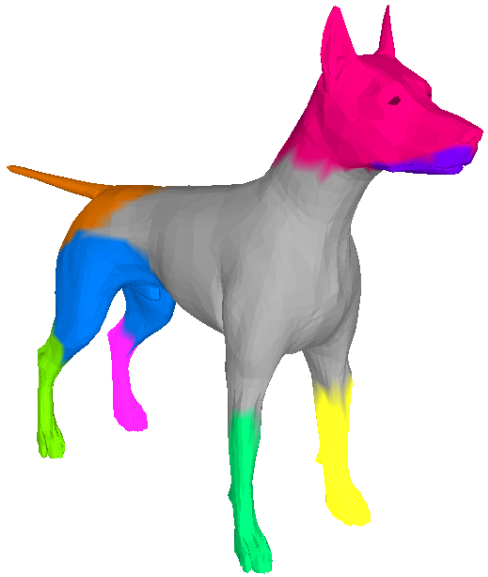
- See (von Luxburg '07) for a detailed analysis.
- The connected components are no longer *disconnected*, but they are only connected by few edges with low weight.

- The Laplacian is a perturbed version of the ideal case.
- Choosing the first k nonzero eigenvalues is easier the larger the eigengap between λ_{k+1} and λ_{k+2}.
- The fact that the first k eigenvectors of the perturbed case are approximately piecewise constant depends on $|\lambda_{k+2} - \lambda_{k+1}|$.
- Choosing k is a crucial issue.

Mesh segmentation using spectral clustering

K=6

K=6



K=9

K=6

Conclusions

- Spectral graph embedding based on the graph Laplacian is a very powerful tool;
- Allows links between graphs and Riemannian manifolds
- There are strong links with Markov chains and random walks
- It allows clustering (or segmentation) under some conditions
- The PERCEPTION group uses it for shape matching, shape segmentation, shape recognition, etc.