MATH 829: Introduction to Data Mining and Analysis
Clustering II

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This lecture is based on U. von Luxburg, *A Tutorial on Spectral Clustering*, Statistics and Computing, 17 (4), 2007.

Spectral clustering: overview

In the previous lecture, we discussed how K-means can be used to cluster points in $\mathbb{R}^p$.

Spectral clustering:

- Very popular clustering method.
- Often outperforms other methods such as K-means.
- Can be used for various "types" of data (not only points in $\mathbb{R}^p$).
- Easy to implement. Only uses basic linear algebra.

Overview of spectral clustering:

1. Construct a *similarity matrix* measuring the similarity of pairs of objects.
2. Use the similarity matrix to construct a (weighted or unweighted) graph.
3. Compute eigenvectors of the *graph Laplacian*.
4. Cluster the graph using the eigenvectors of the graph Laplacian using the K-means algorithm.

Notation

We will use the following notation/conventions:

- $G = (V, E)$ a graph with vertex set $V = \{v_1, \dots, v_n\}$ and edge set $E \subset V \times V$.
- Each edge carries a *weight* $w_{ij} \geq 0$.
- The adjacency matrix of G is $W = W_G = (w_{ij})_{i,j=1}^n$. We will assume W is symmetric (undirected graphs).
- The *degree* of v_i is

$$d_i := \sum_{j=1}^n w_{ij}.$$

- The *degree matrix* of G is $D := \mathrm{diag}(d_1, \dots, d_n)$.
- We denote the complement of $A \subset V$ by $\overline{A}$.
- If $A \subset V$, then we let $\mathbb{1}_A = (f_1, \dots, f_n)^T \in \mathbb{R}^n$, where $f_i = 1$ if $v_i \in A$ and 0 otherwise.

Similarity graphs

- We assume we are given a measure of similarity s between data points $x_1, \dots, x_n \in \mathcal{X}$:

$$s : \mathcal{X} \times \mathcal{X} \to [0, \infty).$$

- We denote by $s_{ij} := s(x_i, x_j)$ the *measure of similarity* between x_i and x_j.
- Equivalently, we may assume we have a measure of *distance* between data points (e.g. $(\mathcal{X}, d)$ is a metric space).
- Let $d_{ij} := d(x_i, x_j)$, the distance between x_i and x_j.
- From d_{ij} (or s_{ij}), we naturally build a *similarity graph*.
- We will discuss 3 popular ways of building a similarity graph.

Similarity graphs (cont.)

Vertex set = $\{v_1, \ldots, v_n\}$ where n is the number of data points.

1. **The ϵ-neighborhood graph:** Connect all points whose pairwise distances are smaller than some $\epsilon > 0$. We usually don't weight the edges. The graph is thus a simple graph (unweighted, undirected graph containing no loops or multiple edges).
2. **The k-nearest neighbor graph:** The goal is to connect v_i to v_j if x_j is among the k nearest neighbords of x_i. However, this leads to a directed graph. We therefore define:
    - the k-nearest neighbor graph: v_i is adjacent to v_j iff x_j is among the k nearest neighbords of x_i **OR** x_i is among the k nearest neighbords of x_j.
    - the mutual k-nearest neighbor graph: v_i is adjacent to v_j iff x_j is among the k nearest neighbords of x_i **AND** x_i is among the k nearest neighbors of x_j.

    We weight the edges by the similarity of their endpoints.

Similarity graphs (cont.)

3. **The fully connected graph:** Connect all points with edge weights s_{ij}. For example, one could use the *Gaussian similarity function* to represent a local neighborhood relationships:

$$s_{ij} = s(x_i, x_j) = \exp(-\|x_i - x_j\|^2/(2\sigma^2)) \qquad (\sigma^2 > 0).$$

   Note: σ^2 controls the width of the neighborhoods.

All graphs mentioned above are regularly used in spectral clustering.

Graph Laplacians

There are three commonly used definitions of the graph Laplacian:

1. **The unnormalized Laplacian** is

$$L := D - W.$$

2. **The normalized symmetric Laplacian** is

$$L_{\text{sym}} := D^{-1/2} L D^{-1/2} = I - D^{-1/2} W D^{-1/2}.$$

3. **The normalized "random walk" Laplacian** is

$$L_{\text{rw}} := D^{-1} L = I - D^{-1} W.$$

We begin by studying properties of the *unnormalized Laplacian*.

The unnormalized Laplacian

Proposition: The matrix L satisfies the following properties:

1. For any $f \in \mathbb{R}^n$:

$$f^T L f = \frac{1}{2} \sum_{i,j=1}^n w_{ij} (f_i - f_j)^2.$$

2. L is symmetric and positive semidefinite.
3. 0 is an eigenvalue of L with associated constant eigenvector $\mathbb{1}$.

Proof: To prove (1),

$$\begin{aligned} f^T L f = f^T D f - f^T W f &= \sum_{i=1}^n d_i f_i^2 - \sum_{i,j=1}^n w_{ij} f_i f_j \\ &= \frac{1}{2} \left(\sum_{i=1}^n d_i f_i^2 - 2 \sum_{i,j=1}^n w_{ij} f_i f_j + \sum_{j=1}^n d_j f_j^2 \right) \\ &= \frac{1}{2} \sum_{i,j=1}^n w_{ij} (f_i - f_j)^2. \end{aligned}$$

(2) follows from (1). (3) is easy. □

The unnormalized Laplacian (cont.)

Proposition: Let G be an undirected graph with non-negative weights. Then:

1. The multiplicity k of the eigenvalue 0 of L equals the number of connected components $A_1, \ldots, A_k$ in the graph.
2. The eigenspace of eigenvalue 0 is spanned by the indicator vectors $\mathbb{1}_{A_1}, \ldots, \mathbb{1}_{A_k}$ of those components.

Proof: If f is an eigenvector associate to $\lambda = 0$, then

$$0 = f^T L f = \sum_{i,j=1}^{n} w_{ij}(f_i - f_j)^2.$$

It follows that $f_i = f_j$ whenever $w_{ij} > 0$. Thus f is constant on the connected components of G. We conclude that the eigenspace of 0 is contained in $\mathrm{span}(\mathbb{1}_{A_1}, \ldots, \mathbb{1}_{A_k})$. Conversely, it is not hard to see that each $\mathbb{1}_{A_i}$ is an eigenvector associated to 0 (write L in block diagonal form). □

The normalized Laplacians

Proposition: The normalized Laplacians satisfy the following properties:

1. For every $f \in \mathbb{R}^n$, we have
$$f^T L_{\mathrm{sym}} f = \frac{1}{2} \sum_{i,j=1}^{n} w_{ij} \left(\frac{f_i}{\sqrt{d_i}} - \frac{f_j}{\sqrt{d_j}} \right)^2.$$
2. λ is an eigenvalue of L_{rw} with eigenvector u if and only if λ is an eigenvalue of L_{sym} with eigenvector $w = D^{1/2}u$.
3. λ is an eigenvalue of L_{rw} with eigenvector u if and only if λ and u solve the generalized eigenproblem $Lu = \lambda D u$.

Proof: The proof of (1) is similar to the proof of the analogous result for the unnormalized Laplacian. (2) and (3) follow easily by using appropriate rescalings.

The normalized Laplacians (cont.)

Proposition: Let G be an undirected graph with non-negative weights. Then:

1. The multiplicity k of the eigenvalue 0 of both L_{sym} and L_{rw} equals the number of connected components $A_1, \ldots, A_k$ in the graph.
2. For L_{rw}, the eigenspace of eigenvalue 0 is spanned by the indicator vectors $\mathbb{1}_{A_i}$, $i = 1, \ldots, k$.
3. For L_{sym}, the eigenspace of eigenvalue 0 is spanned by the vectors $D^{1/2}\mathbb{1}_{A_i}$, $i = 1, \ldots, k$.

Proof: Similar to the proof of the analogous result for the unnormalized Laplacian.