# MATH 567: Mathematical Techniques in Data Science
# Clustering II

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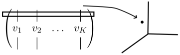
This lecture is based on U. von Luxburg, *A Tutorial on Spectral Clustering*, Statistics and Computing, 17 (4), 2007.

## Spectral clustering: overview

Overview of spectral clustering:

1. Construct a *similarity matrix* measuring the similarity of pairs of objects (e.g. $s_{ij} = \exp(-\|x_i - x_j\|^2/(2\sigma^2))$).
2. Use the similarity matrix to construct a (weighted or unweighted) graph.
3. Compute eigenvectors of the (normalized or unnormalized) *graph Laplacian*:
$$L = D - W, \qquad L_{\text{sym}} = D^{-1/2} L D^{-1/2}.$$
4. Construct a matrix containing the first $K$ eigenvectors of $L$ or $L_{\text{sym}}$ as columns.
5. Each row identifies a vertex of the graph to a point in $\mathbb{R}^K$.

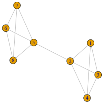



6. Cluster those points using the $K$-means algorithm.



## Example

Let us try to cluster the following graph:




$$A = \begin{pmatrix} 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \end{pmatrix}, \qquad L = \begin{pmatrix} 3 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 4 & -1 & -1 & -1 & 0 & 0 & 0 \\ -1 & -1 & 3 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & -1 & 3 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 4 & -1 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 3 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & -1 & 3 & -1 \\ 0 & 0 & 0 & 0 & -1 & -1 & -1 & 3 \end{pmatrix}$$

We have:

$$v_2 = (-0.3825277, -0.2470177, -0.3825277, -0.3825277, 0.2470177, 0.3825277, 0.3825277, 0.3825277)^T.$$



## 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 associated 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). $\square$



## 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. $\lambda$ is an eigenvalue of $L_{\mathrm{rw}}$ with eigenvector $u$ if and only if $\lambda$ is an eigenvalue of $L_{\mathrm{sym}}$ with eigenvector $w = D^{1/2}u$.
3. $\lambda$ is an eigenvalue of $L_{\mathrm{rw}}$ with eigenvector $u$ if and only if $\lambda$ 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.)

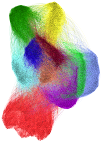
**Proposition:** Let $G$ be an undirected graph with non-negative weights. Then:

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



## Graph cuts



- $G$ graph with (weighted) adjacency matrix $W = (w_{ij})$.
- We define:

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

- $|A| :=$ number of vertices in $A$.
- $\mathrm{vol}(A) := \sum_{i \in A} d_i$.

Given a partition $A_1, \ldots, A_k$ of the vertices of $G$, we let

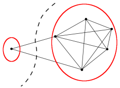
$$\mathrm{cut}(A_1, \ldots, A_k) := \frac{1}{2} \sum_{i=1}^{k} W(A_i, \overline{A}_i).$$

The min-cut problem consists of solving:

$$\min_{\substack{V = A_1 \cup \cdots \cup A_k \\ A_i \cap A_j = \emptyset \ \forall i \neq j}} \mathrm{cut}(A_1, \ldots, A_k).$$

## Graph cuts (cont.)

- The min-cut problem can be solved efficiently when $k = 2$ (see Stoer and Wagner 1997).
- In practice it often does not lead to satisfactory partitions.
- In many cases, the solution of min-cut simply separates one individual vertex from the rest of the graph.



- We would like clusters to have a reasonably large number of points.
- We therefore modify the min-cut problem to enforce such constraints.



## Balanced cuts

The two most common objective functions that are used as a replacement to the min-cut objective are:

1. RatioCut (Hagen and Kahng, 1992):

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

2. Normalized cut (Shi and Malik, 2000):

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

- Note: both objective functions take larger values when the clusters $A_i$ are "small".
- Resulting clusters are more "balanced".
- However, the resulting problems are NP hard - see Wagner and Wagner (1993).



## Spectral clustering

Spectral clustering provides a way to *relax* the RatioCut and the Normalized cut problems.

Strategy:

1. Express the original problem as a linear algebra problem involving discrete/combinatorial constraints.
2. Relax/remove the constraints.

**RatioCut** with $k = 2$: solve

$$\min_{A \subset V} \text{RatioCut}(A, \overline{A}).$$

Given $A \subset V$, let $f \in \mathbb{R}^n$ be given by

$$f_i := \begin{cases} \sqrt{|\overline{A}|/|A|} & \text{if } v_i \in A \\ -\sqrt{|A|/|\overline{A}|} & \text{if } v_i \notin A. \end{cases}$$



## Relaxing RatioCut

Let $L = D - W$ be the (unnormalized) Laplacian of $G$. Then

$$\begin{aligned}
f^T L f &= \frac{1}{2}\sum_{i,j=1}^{n} w_{ij}(f_i - f_j)^2 \\
&= \frac{1}{2}\sum_{i \in A, j \in \overline{A}} w_{ij}\left(\sqrt{\frac{|\overline{A}|}{|A|}} + \sqrt{\frac{|A|}{|\overline{A}|}}\right)^2 + \frac{1}{2}\sum_{i \in \overline{A}, j \in A} w_{ij}\left(-\sqrt{\frac{|\overline{A}|}{|A|}} - \sqrt{\frac{|A|}{|\overline{A}|}}\right)^2 \\
&= W(A, \overline{A})\left(2 + \frac{|\overline{A}|}{|A|} + \frac{|A|}{|\overline{A}|}\right) \\
&= W(A, \overline{A})\left(\frac{|A| + |\overline{A}|}{|A|} + \frac{|A| + |\overline{A}|}{|\overline{A}|}\right) \\
&= |V| \cdot \frac{1}{2}\left(\frac{W(A, \overline{A})}{|A|} + \frac{W(\overline{A}, A)}{|\overline{A}|}\right) \\
&= |V| \cdot \text{RatioCut}(A, \overline{A}).
\end{aligned}$$

since $|A| + |\overline{A}| = |V|$, and $W(A, \overline{A}) = W(\overline{A}, A)$.

## Relaxing RatioCut (cont.)

- We showed:

$$f^T L f = \frac{1}{2} \sum_{i,j=1}^{n} w_{ij}(f_i - f_j)^2 = |V| \cdot \text{RatioCut}(A, \overline{A}).$$

- Moreover, note that

$$\sum_{i=1}^{n} f_i = \sum_{i \in A} \sqrt{\frac{|\overline{A}|}{|A|}} - \sum_{i \in \overline{A}} \sqrt{\frac{|A|}{|\overline{A}|}} = |A| \cdot \sqrt{\frac{|\overline{A}|}{|A|}} - |\overline{A}| \cdot \sqrt{\frac{|A|}{|\overline{A}|}} = 0.$$

Thus $f \perp \mathbb{1}$.

- Finally,

$$\|f\|_2^2 = \sum_{i=1}^{n} f_i^2 = |A| \cdot \frac{|\overline{A}|}{|A|} + |\overline{A}| \cdot \frac{|A|}{|\overline{A}|} = |V| = n.$$

Thus, we have showed that the Ratio-Cut problem is equivalent to

$$\min_{A \subset V} f^T L f$$
$$\text{subject to } f \perp \mathbb{1}, \|f\| = \sqrt{n}, f_i \text{ defined as above.}$$



## Relaxing RatioCut (cont.)

We have:

$$\min_{A \subset V} f^T L f$$
$$\text{subject to } f \perp \mathbb{1}, \|f\| = \sqrt{n}, f_i \text{ defined as above.}$$

- This is a discrete optimization problem since the entries of $f$ can only take two values: $\sqrt{|\overline{A}|/|A|}$ and $-\sqrt{|A|/|\overline{A}|}$.
- The problem is NP hard.

The natural relaxation of the problem is to **remove the discreteness condition** on $f$ and solve

$$\min_{f \in \mathbb{R}^n} f^T L f$$
$$\text{subject to } f \perp \mathbb{1}, \|f\| = \sqrt{n}.$$



## Relaxing RatioCut (cont.)

- Using properties of the Rayleigh quotient, it is not hard to show that the solution of

$$\min_{f \in \mathbb{R}^n} f^T L f$$
$$\text{subject to } f \perp \mathbb{1}, \|f\| = \sqrt{n}.$$

is an eigenvector of $L$ corresponding to the second eigenvalue.

- Clearly, if $\tilde{f}$ is the solution of the problem, then

$$\tilde{f}^T L \tilde{f} \leq \min_{A \subset V} \text{RatioCut}(A, \overline{A}).$$

- How do we get the clusters from $\tilde{f}$?
- We could set

$$\begin{cases} v_i \in A & \text{if } f_i \geq 0 \\ v_i \in \overline{A} & \text{if } f_i < 0. \end{cases}$$

- More generally, we *cluster* the coordinates of $f$ using $K$-means. This is the **unnormalized spectral clustering algorithm** for $k = 2$.
- The above process can be generalized to $k \geq 2$ clusters.



## Unnormalized spectral clustering: summary

The **unnormalized spectral clustering algorithm**:

**Unnormalized spectral clustering**

Input: Similarity matrix $S \in \mathbb{R}^{n \times n}$, number $k$ of clusters to construct.
- Construct a similarity graph by one of the ways described in Section 2. Let $W$ be its weighted adjacency matrix.
- Compute the unnormalized Laplacian $L$.
- **Compute the first $k$ eigenvectors $u_1, \ldots, u_k$ of $L$.**
- Let $U \in \mathbb{R}^{n \times k}$ be the matrix containing the vectors $u_1, \ldots, u_k$ as columns.
- For $i = 1, \ldots, n$, let $y_i \in \mathbb{R}^k$ be the vector corresponding to the $i$-th row of $U$.
- Cluster the points $(y_i)_{i=1,\ldots,n}$ in $\mathbb{R}^k$ with the $k$-means algorithm into clusters $C_1, \ldots, C_k$.

Output: Clusters $A_1, \ldots, A_k$ with $A_i = \{j | \, y_j \in C_i\}$.

Source: von Luxburg, 2007.

## Normalized spectral clustering

- Relaxing the RatioCut leads to unnormalized spectral clustering.
- By relaxing the Ncut problem, we obtain the **Normalized spectral clustering** algorithm of Shi and Malik (2000).

**Normalized spectral clustering according to Shi and Malik (2000)**

Input: Similarity matrix $S \in \mathbb{R}^{n \times n}$, number $k$ of clusters to construct.
- Construct a similarity graph by one of the ways described in Section 2. Let $W$ be its weighted adjacency matrix.
- Compute the unnormalized Laplacian $L$.
- **Compute the first $k$ generalized eigenvectors $u_1, \dots, u_k$ of the generalized eigenproblem $Lu = \lambda Du$.**
- Let $U \in \mathbb{R}^{n \times k}$ be the matrix containing the vectors $u_1, \dots, u_k$ as columns.
- For $i = 1, \dots, n$, let $y_i \in \mathbb{R}^k$ be the vector corresponding to the $i$-th row of $U$.
- Cluster the points $(y_i)_{i=1,\dots,n}$ in $\mathbb{R}^k$ with the $k$-means algorithm into clusters $C_1, \dots, C_k$.

Output: Clusters $A_1, \dots, A_k$ with $A_i = \{j \mid y_j \in C_i\}$.

Source: von Luxburg, 2007.

- Note: The solutions of $Lu = \lambda Du$ are the eigenvectors of $L_{\text{rw}}$.

See von Luxburg (2007) for details.



## The normalized clustering algorithm of Ng et al.

- Another popular variant of the spectral clustering algorithm was provided by Ng, Jordan, and Weiss (2002).
- The algorithm uses $L_{\text{sym}}$ instead of $L$ (unnormalized clustering) or $L_{\text{rw}}$ (Shi and Malik's normalized clustering).

**Normalized spectral clustering according to Ng, Jordan, and Weiss (2002)**

Input: Similarity matrix $S \in \mathbb{R}^{n \times n}$, number $k$ of clusters to construct.
- Construct a similarity graph by one of the ways described in Section 2. Let $W$ be its weighted adjacency matrix.
- Compute the normalized Laplacian $L_{\text{sym}}$.
- **Compute the first $k$ eigenvectors $u_1, \dots, u_k$ of $L_{\text{sym}}$.**
- Let $U \in \mathbb{R}^{n \times k}$ be the matrix containing the vectors $u_1, \dots, u_k$ as columns.
- **Form the matrix $T \in \mathbb{R}^{n \times k}$ from $U$ by normalizing the rows to norm 1,** that is set $t_{ij} = u_{ij} / (\sum_k u_{ik}^2)^{1/2}$.
- For $i = 1, \dots, n$, let $y_i \in \mathbb{R}^k$ be the vector corresponding to the $i$-th row of $T$.
- Cluster the points $(y_i)_{i=1,\dots,n}$ with the $k$-means algorithm into clusters $C_1, \dots, C_k$.

Output: Clusters $A_1, \dots, A_k$ with $A_i = \{j \mid y_j \in C_i\}$.

Source: von Luxburg, 2007.

See von Luxburg (2007) for details.