

Randomised Algorithms

Lecture 11: Spectral Graph Theory

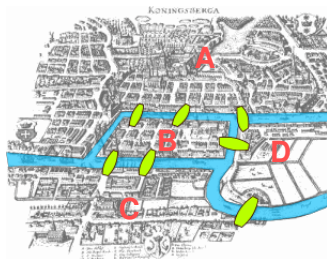
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Introduction to (Spectral) Graph Theory and Clustering

Matrices, Spectrum and Structure

A Simplified Clustering Problem

Origin of Graph Theory



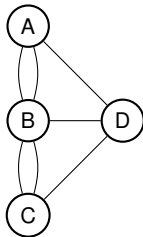
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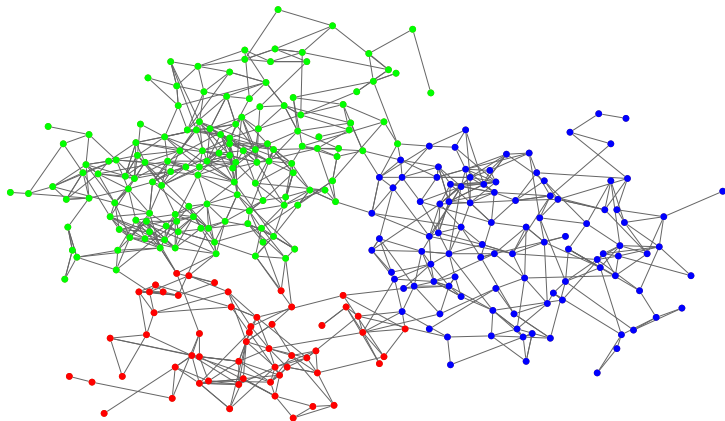
Seven Bridges at Königsberg 1737

Leonhard Euler (1707-1783)



Is there a tour which crosses each bridge **exactly once**?

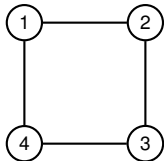
Graphs Nowadays: Clustering



Goal: Use spectrum of graphs (unstructured data) to extract clustering (communities) or other structural information.

- Applications of Graph Clustering
 - Community detection
 - Group webpages according to their topics
 - Find proteins performing the same function within a cell
 - Image segmentation
 - Identify bottlenecks in a network
 - ...
- **Unsupervised** learning method
(there is no ground truth (usually), and we cannot learn from mistakes!)
- Different formalisations for different applications
 - **Geometric Clustering**: partition points in a Euclidean space
 - k -means, k -medians, k -centres, etc.
 - **Graph Clustering**: partition vertices in a graph
 - modularity, **conductance**, min-cut, etc.

Graphs



- Connectivity
- Bipartiteness
- Number of triangles
- Graph Clustering
- Graph isomorphism
- Maximum Flow
- Shortest Paths
- ...

Matrices

$$\begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

- Eigenvalues
- Eigenvectors
- Inverse
- Determinant
- Matrix-powers
- ...

Outline

Introduction to (Spectral) Graph Theory and Clustering

Matrices, Spectrum and Structure

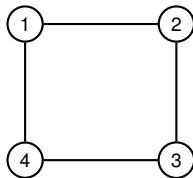
A Simplified Clustering Problem

Adjacency Matrix

Adjacency matrix

Let $G = (V, E)$ be an undirected graph. The adjacency matrix of G is the n by n matrix \mathbf{A} defined as

$$\mathbf{A}_{u,v} = \begin{cases} 1 & \text{if } \{u, v\} \in E \\ 0 & \text{otherwise.} \end{cases}$$



$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

Properties of \mathbf{A} :

- The sum of elements in each row/column i equals the degree of the corresponding vertex i , $\deg(i)$
- Since G is undirected, \mathbf{A} is symmetric

Eigenvalues and Graph Spectrum of A

Eigenvalues and Eigenvectors

Let $\mathbf{M} \in \mathbb{R}^{n \times n}$, $\lambda \in \mathbb{C}$ is an **eigenvalue** of \mathbf{M} if and only if there exists $x \in \mathbb{R}^n \setminus \{\mathbf{0}\}$ such that

$$\mathbf{M}x = \lambda x.$$

We call x an **eigenvector** of \mathbf{M} corresponding to the eigenvalue λ .

An **undirected** graph G is **d -regular** if every degree is d , i.e., every vertex has exactly d connections.

Graph Spectrum

Let \mathbf{A} be the adjacency matrix of a **d -regular** graph G with n vertices. Then, \mathbf{A} has n real eigenvalues $\lambda_1 \leq \dots \leq \lambda_n$ and n corresponding **orthonormal eigenvectors** f_1, \dots, f_n . These eigenvalues associated with their **multiplicities** constitute the **spectrum** of G .

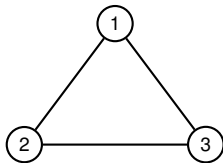
For **symmetric** matrices: **algebraic multiplicity** = **geometric multiplicity**

Example 1

Bonus: Can you find a short-cut to $\det(\mathbf{A} - \lambda \cdot \mathbf{I})$?



Exercise: What are the Eigenvalues and Eigenvectors?



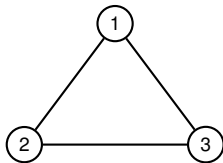
$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

Example 1

Bonus: Can you find a short-cut to $\det(\mathbf{A} - \lambda \cdot \mathbf{I})$?



Exercise: What are the Eigenvalues and Eigenvectors?



$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

Solution:

- The three eigenvalues are $\lambda_1 = \lambda_2 = -1, \lambda_3 = 2$.
- The three eigenvectors are (for example):

$$f_1 = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \quad f_2 = \begin{pmatrix} -\frac{1}{2} \\ 1 \\ -\frac{1}{2} \end{pmatrix}, \quad f_3 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}.$$

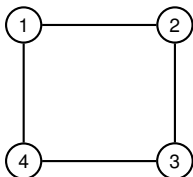
Laplacian Matrix

Laplacian Matrix

Let $G = (V, E)$ be a d -regular undirected graph. The (normalised) Laplacian matrix of G is the n by n matrix \mathbf{L} defined as

$$\mathbf{L} = \mathbf{I} - \frac{1}{d}\mathbf{A},$$

where \mathbf{I} is the $n \times n$ identity matrix.



$$\mathbf{L} = \begin{pmatrix} 1 & -1/2 & 0 & -1/2 \\ -1/2 & 1 & -1/2 & 0 \\ 0 & -1/2 & 1 & -1/2 \\ -1/2 & 0 & -1/2 & 1 \end{pmatrix}$$

Properties of \mathbf{L} :

- The sum of elements in each row/column equals zero
- \mathbf{L} is symmetric

Relating Spectrum of Adjacency Matrix and Laplacian Matrix

Correspondence between Adjacency and Laplacian Matrix

A and **L** have the same eigenvectors.



Exercise: Prove this correspondence. Hint: Use that $\mathbf{L} = \mathbf{I} - \frac{1}{d}\mathbf{A}$.

Eigenvalues and Graph Spectrum of L

Eigenvalues and eigenvectors

Let $\mathbf{M} \in \mathbb{R}^{n \times n}$, $\lambda \in \mathbb{C}$ is an **eigenvalue** of \mathbf{M} if and only if there exists $x \in \mathbb{R}^n \setminus \{\mathbf{0}\}$ such that

$$\mathbf{M}x = \lambda x.$$

We call x an **eigenvector** of \mathbf{M} corresponding to the eigenvalue λ .

Graph Spectrum

Let \mathbf{L} be the **Laplacian matrix** of a d -regular graph G with n vertices. Then, \mathbf{L} has n real eigenvalues $\lambda_1 \leq \dots \leq \lambda_n$ and n corresponding orthonormal eigenvectors f_1, \dots, f_n .

Useful Facts of Graph Spectrum

Lemma

Let \mathbf{L} be the Laplacian matrix of an undirected, regular graph $G = (V, E)$ with eigenvalues $\lambda_1 \leq \dots \leq \lambda_n$.

1. $\lambda_1 = 0$ with eigenvector $\mathbf{1}$
2. the multiplicity of the eigenvalue 0 is equal to the number of connected components in G
3. $\lambda_n \leq 2$
4. $\lambda_n = 2$ iff there exists a bipartite connected component.

The proof of these properties is based on a powerful characterisation of eigenvalues/vectors!

A Min-Max Characterisation of Eigenvalues and Eigenvectors

Courant-Fischer Min-Max Formula

Let \mathbf{M} be an n by n symmetric matrix with eigenvalues $\lambda_1 \leq \dots \leq \lambda_n$.
Then,

$$\lambda_k = \min_{\substack{x^{(1)}, \dots, x^{(k)} \in \mathbb{R}^n \setminus \{\mathbf{0}\}, \\ x^{(i)} \perp x^{(j)}}} \max_{i \in \{1, \dots, k\}} \frac{x^{(i)T} \mathbf{M} x^{(i)}}{x^{(i)T} x^{(i)}}.$$

The eigenvectors corresponding to $\lambda_1, \dots, \lambda_k$ minimise such expression.

$$\lambda_1 = \min_{x \in \mathbb{R}^n \setminus \{\mathbf{0}\}} \frac{x^T \mathbf{M} x}{x^T x}$$

minimised by an eigenvector f_1 for λ_1

$$\lambda_2 = \min_{\substack{x \in \mathbb{R}^n \setminus \{\mathbf{0}\} \\ x \perp f_1}} \frac{x^T \mathbf{M} x}{x^T x}$$

minimised by f_2

Quadratic Forms of the Laplacian

Lemma

Let \mathbf{L} be the Laplacian matrix of a d -regular graph $G = (V, E)$ with n vertices. For any $x \in \mathbb{R}^n$,

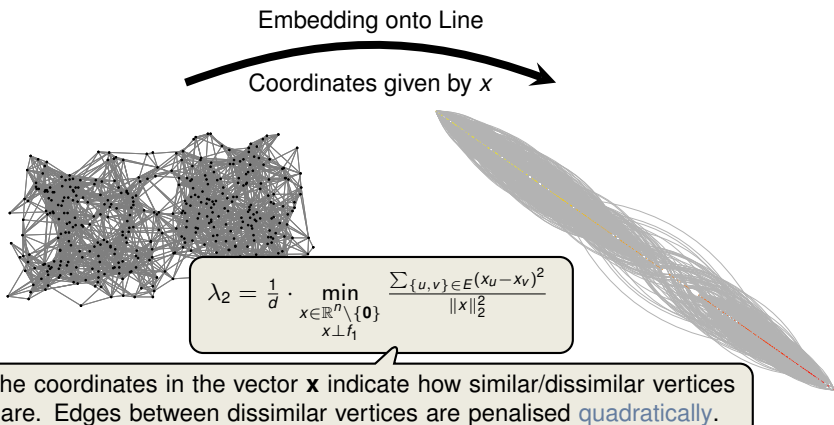
$$x^T \mathbf{L} x = \sum_{\{u,v\} \in E} \frac{(x_u - x_v)^2}{d}.$$

Proof:

$$\begin{aligned} x^T \mathbf{L} x &= x^T \left(\mathbf{I} - \frac{1}{d} \mathbf{A} \right) x = x^T x - \frac{1}{d} x^T \mathbf{A} x \\ &= \sum_{u \in V} x_u^2 - \frac{2}{d} \sum_{\{u,v\} \in E} x_u x_v \\ &= \frac{1}{d} \sum_{\{u,v\} \in E} (x_u^2 + x_v^2 - 2x_u x_v) \\ &= \sum_{\{u,v\} \in E} \frac{(x_u - x_v)^2}{d}. \end{aligned}$$

Visualising a Graph

Question: How can we visualize a complicated object like an unknown graph with many vertices in low-dimensional space?



Outline

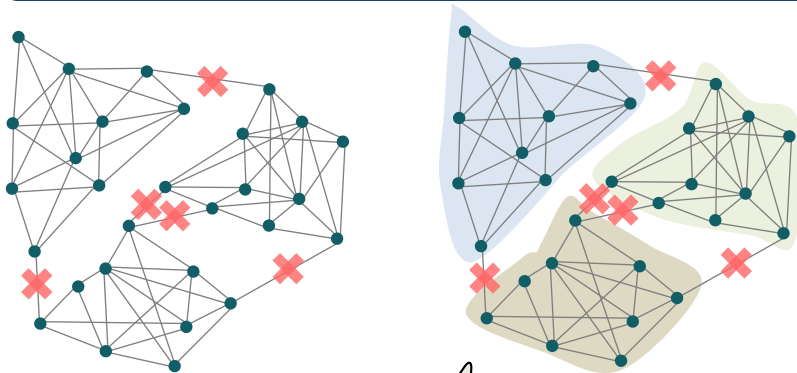
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A Simplified Clustering Problem

Partition the graph into **connected components** so that any pair of vertices in the same component is connected, but vertices in different components are not.

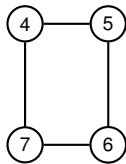
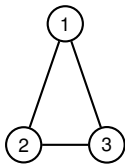


We could obviously solve this easily using DFS/BFS, but let's see how we can tackle this using the **spectrum of L** !

Example 2



Exercise: What are the Eigenvectors with Eigenvalue 0 of \mathbf{L} ?



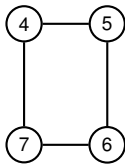
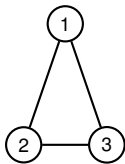
$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \end{pmatrix}$$

$$\mathbf{L} = \begin{pmatrix} 1 & -\frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 & 0 \\ -\frac{1}{2} & 1 & -\frac{1}{2} & 0 & 0 & 0 & 0 \\ -\frac{1}{2} & -\frac{1}{2} & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -\frac{1}{2} & 0 & -\frac{1}{2} \\ 0 & 0 & 0 & -\frac{1}{2} & 1 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{2} & 1 & -\frac{1}{2} \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & -\frac{1}{2} & 1 \end{pmatrix}$$

Example 2



Exercise: What are the Eigenvectors with Eigenvalue 0 of L ?



$$A = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \end{pmatrix}$$

$$L = \begin{pmatrix} 1 & -\frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 & 0 \\ -\frac{1}{2} & 1 & -\frac{1}{2} & 0 & 0 & 0 & 0 \\ -\frac{1}{2} & -\frac{1}{2} & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -\frac{1}{2} & 0 & -\frac{1}{2} \\ 0 & 0 & 0 & -\frac{1}{2} & 1 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{2} & 1 & -\frac{1}{2} \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & -\frac{1}{2} & 1 \end{pmatrix}$$

Solution:

- The two smallest eigenvalues are $\lambda_1 = \lambda_2 = 0$.
- The corresponding two eigenvectors are:

$$f_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad f_2 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \quad (\text{or } f_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \quad f_2 = \begin{pmatrix} -1/3 \\ -1/3 \\ -1/3 \\ 1/4 \\ 1/4 \\ 1/4 \\ 1/4 \end{pmatrix})$$

Thus we can easily solve the simplified clustering problem by computing the eigenvectors with eigenvalue

Next Lecture: A fine-grained approach works even if the clusters are **sparsely** connected!

Proof of Lemma, 2nd statement (non-examinable)

Let us generalise and formalise the previous example!

Proof (multiplicity of 0 equals the no. of connected components):

1. (“ \implies ” $cc(G) \leq \text{mult}(0)$). We will show:

G has exactly k connected comp. $C_1, \dots, C_k \implies \lambda_1 = \dots = \lambda_k = 0$

- Take $\chi_{C_i} \in \{0, 1\}^n$ such that $\chi_{C_i}(u) = \mathbf{1}_{u \in C_i}$ for all $u \in V$
- Clearly, the χ_{C_i} 's are orthogonal
- $\chi_{C_i}^T L \chi_{C_i} = \frac{1}{d} \cdot \sum_{\{u,v\} \in E} (\chi_{C_i}(u) - \chi_{C_i}(v))^2 = 0 \implies \lambda_1 = \dots = \lambda_k = 0$

2. (“ \impliedby ” $cc(G) \geq \text{mult}(0)$). We will show:

$\lambda_1 = \dots = \lambda_k = 0 \implies G$ has at least k connected comp. C_1, \dots, C_k

- there exist f_1, \dots, f_k orthonormal such that $\sum_{\{u,v\} \in E} (f_i(u) - f_i(v))^2 = 0$
- $\implies f_1, \dots, f_k$ constant on connected components
- as f_1, \dots, f_k are pairwise orthogonal, G must have k different connected components.

□