Randomised Algorithms

Lecture 11: Spectral Graph Theory

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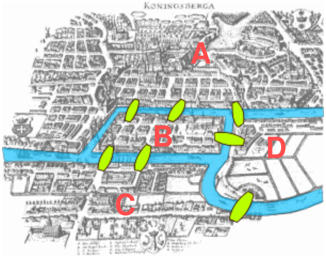
Outline

Introduction to (Spectral) Graph Theory and Clustering

Matrices, Spectrum and Structure

A Simplified Clustering Problem

Origin of Graph Theory

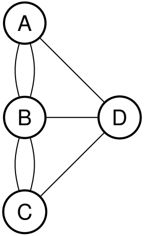


Source: Wikipedia

Seven Bridges at Königsberg 1737

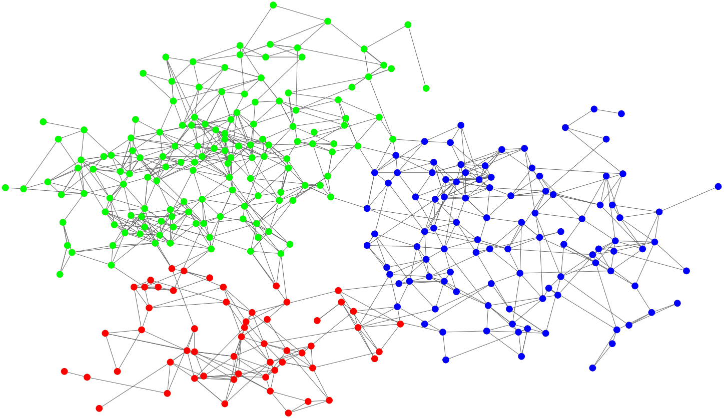
Source: Wikipedia

Leonhard Euler (1707-1783)



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

Graphs Nowadays: Clustering



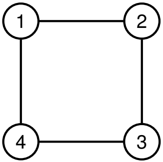
Goal: Use spectrum of graphs (unstructured data) to extract clustering (communitites) or other structural information.

Graph Clustering (applications)

- 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 and Matrices

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
- ...

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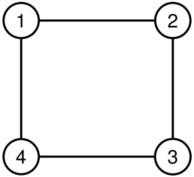
Adjacency Matrix

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 $x \in \mathbb{C}^n \setminus \{\mathbf{0}\}$ 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 $\lambda_1 \leq \cdots \leq \lambda_n$ and n corresponding orthonormal eigenvectors $f_1, \ldots, f_n$. These eigenvalues associated with their multiplicities constitute the spectrum of G.

$=$ orthogonal and normalised

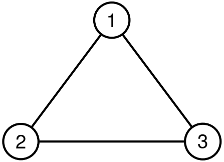
Remark: For symmetric matrices we have algebraic multiplicity $=$ geometric multiplicity (otherwise $\geq$)

Example 1

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

???

Question: What are the Eigenvalues and Eigenvectors?



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

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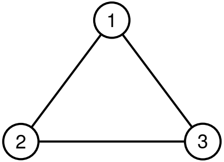

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

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.

???

Question: What is the matrix $\frac{1}{d} \cdot \mathbf{A}$?

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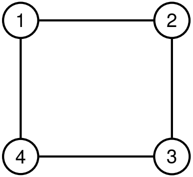

$$\mathbf{L} = \begin{pmatrix} 1 & -1/2 & 0 & -1/2 \\ -1/2 & 1 & -1/2 & 0 \\ 0 & -1/2 & 1 & -1/2 \\ -1/2 & 0 & -1/2 & 1 \end{pmatrix}$$

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 set of eigenvectors.

Exercise: Prove this correspondence. Hint: Use that $\mathbf{L} = \mathbf{I} - \frac{1}{d}\mathbf{A}$.
[Exercise 11/12.1]

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 $x \in \mathbb{C}^n \setminus \{\mathbf{0}\}$ such that

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Useful Facts of Graph Spectrum

Lemma

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

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 $\lambda_1 \leq \cdots \leq \lambda_n$. Then,

$$\lambda_k = \min_{S:\ \dim(S)=k} \max_{x \in S, x \neq \mathbf{0}} \frac{x^{(i)^T} \mathbf{M} x^{(i)}}{x^{(i)^T} x^{(i)}},$$

where S is a subspace of $\mathbb{R}^n$. The eigenvectors corresponding to $\lambda_1, \ldots, \lambda_k$ 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:

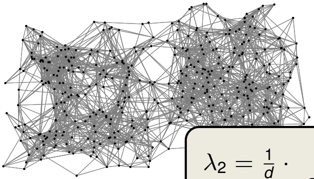
$$\begin{aligned}
x^T \mathbf{L} x = x^T \left(\mathbf{I} - \frac{1}{d} \mathbf{A} \right) x &= x^T x - \frac{1}{d} x^T \mathbf{A} x \\
&= \sum_{u \in V} x_u^2 - \frac{2}{d} \sum_{\{u,v\} \in E} x_u x_v \\
&= \frac{1}{d} \sum_{\{u,v\} \in E} (x_u^2 + x_v^2 - 2 x_u x_v) \\
&= \sum_{\{u,v\} \in E} \frac{(x_u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

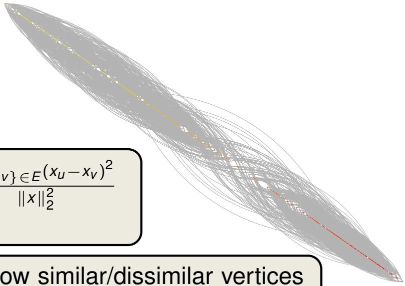
Visualising a Graph

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

Embedding onto Line

Coordinates given by x





$$\lambda_2 = \frac{1}{d} \cdot \min_{\substack{x \in \mathbb{R}^n \setminus \{\mathbf{0}\} \\ x \perp f_1}} \frac{\sum_{\{u,v\} \in E} (x_u - x_v)^2}{\|x\|_2^2}$$

The coordinates in the vector **x** indicate how similar/dissimilar vertices are. Edges between dissimilar vertices are penalised quadratically.

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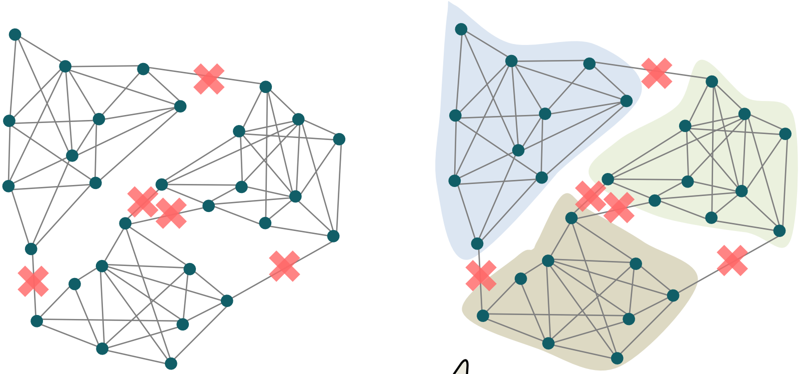
A Simplified Clustering Problem

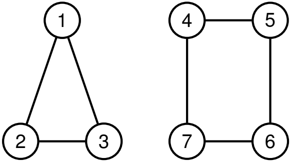
Partition the graph into ***connected components*** *so that any pair of vertices in the same component is connected, but vertices in different components are not.*



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

Question: What are the Eigenvectors with Eigenvalue 0 of **L**?

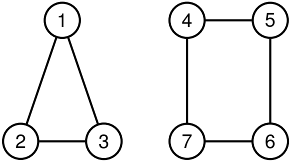


$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \end{pmatrix}$$

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

Example 2

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



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

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

Solution:

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

Thus we can easily solve the simplified clustering problem by computing the eigenvectors with eigenvalue 0

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

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. ("$\Longrightarrow$" $cc(G) \leq \mathrm{mult}(0)$). We will show:
   G has exactly k connected comp. $C_1, \ldots, C_k \quad \Rightarrow \quad \lambda_1 = \cdots = \lambda_k = 0$
   - 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
   - $\chi_{C_i}^T \mathbf{L} \chi_{C_i} = \frac{1}{d} \cdot \sum_{\{u,v\} \in E} (\chi_{C_i}(u) - \chi_{C_i}(v))^2 = 0 \quad \Rightarrow \quad \lambda_1 = \cdots = \lambda_k = 0$

2. ("$\Longleftarrow$" $cc(G) \geq \mathrm{mult}(0)$). We will show:
   $\lambda_1 = \cdots = \lambda_k = 0 \quad \Rightarrow \quad G$ has at least k connected comp. $C_1, \ldots, C_k$
   - there exist $f_1, \ldots, f_k$ orthonormal such that $\sum_{\{u,v\} \in E} (f_i(u) - f_i(v))^2 = 0$
   - $\Rightarrow f_1, \ldots, f_k$ constant on connected components
   - as $f_1, \ldots, f_k$ are pairwise orthogonal, G must have k different connected components.

$\square$