Randomised Algorithms

Lecture 11-12: Spectral Graph Theory and Clustering

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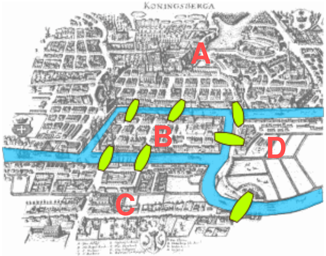
Outline

Origin of Graph Theory



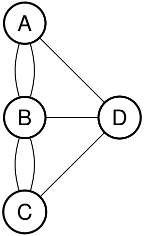
Source: Wikipedia

Seven Bridges at Königsberg 1737

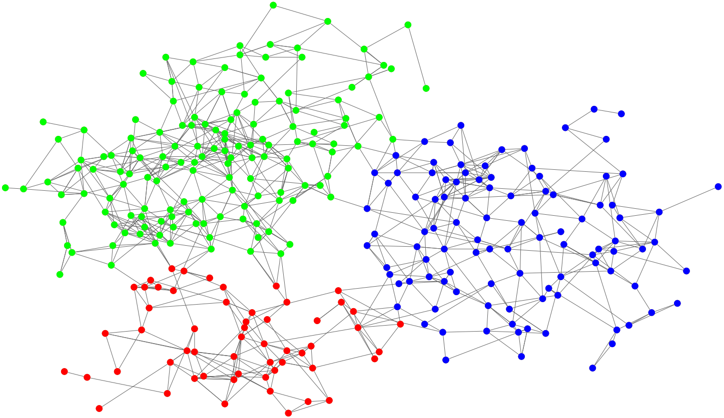
Source: Wikipedia

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)

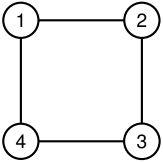
- Applications of Graph Clustering
  - Community detection
  - Group webpages according to their topics
  - Find proteins performing the same function within a cell
  - Image segmentation
  - Identify bottlenecks in a network
  - ...
- Unsupervised learning method
  (there is no ground truth (usually), 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
- ...

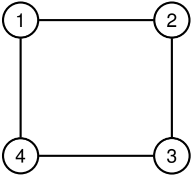
Outline

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

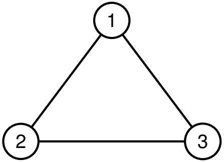
Let $\mathbf{A}$ be the adjacency matrix of a d-regular graph G with n vertices. Then, $\mathbf{A}$ has n real eigenvalues $\lambda_1 \leq \cdots \leq \lambda_n$ and n corresponding orthonormal eigenvectors $f_1, \ldots, f_n$. These eigenvalues associated with their multiplicities constitute the spectrum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

For symmetric matrices: algebraic multiplicity = geometric multiplicity

Exercise 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):

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

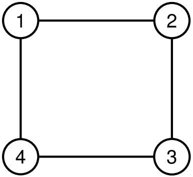
Laplacian Matrix

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

$\mathbf{A}$ and $\mathbf{L}$ have the same eigenvectors.

Proof:

- Let λ and f be an eigenvalue and eigenvector of $\mathbf{A}$, i.e., $\mathbf{A} \cdot f = \lambda \cdot f$.
- Then:

$$\begin{aligned} \mathbf{L} \cdot f &= \left(\mathbf{I} - \frac{1}{d} \mathbf{A} \right) \cdot f \\ &= \mathbf{I} \cdot f - \frac{1}{d} \mathbf{A} \cdot f \\ &= f - \frac{1}{d} \lambda \cdot f \\ &= \left(1 - \frac{\lambda}{d} \right) \cdot f. \end{aligned}$$

- Hence $(1 - \frac{\lambda}{d}, f)$ is an eigenvalue and eigenvector pair of $\mathbf{L}$. □

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

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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 $\lambda_1 \leq \cdots \leq \lambda_n$ and n corresponding orthonormal eigenvectors $f_1, \ldots, f_n$.

Useful Facts of Graph Spectrum

Lemma

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

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,

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

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:

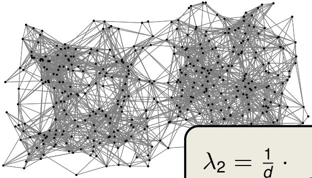
$$\begin{aligned} x^T \mathbf{L} x = x^T \left(\mathbf{I} - \frac{1}{d} \mathbf{A} \right) x &= x^T x - \frac{1}{d} x^T \mathbf{A} x \\ &= \sum_{u \in V} x_u^2 - \frac{2}{d} \sum_{\{u,v\} \in E} x_u x_v \\ &= \frac{1}{d} \sum_{\{u,v\} \in E} (x_u^2 + x_v^2 - 2 x_u x_v) \\ &= \sum_{\{u,v\} \in E} \frac{(x_u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

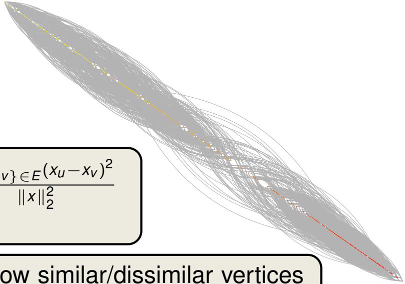
Visualising a Graph

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





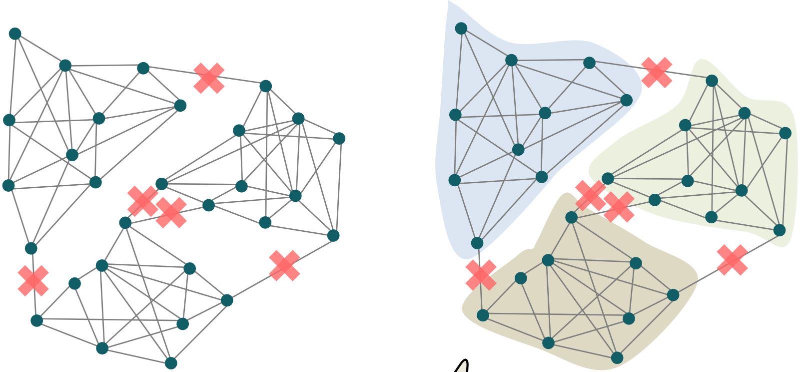
$$\lambda_2 = \frac{1}{d} \cdot \min_{\substack{x \in \mathbb{R}^n \setminus \{\mathbf{0}\} \\ x \perp f_1}} \frac{\sum_{\{u,v\} \in E} (x_u - x_v)^2}{\|x\|_2^2}$$

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

Outline

A Simplified Clustering Problem

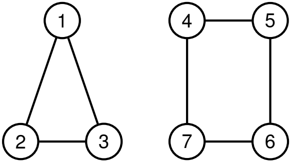
*Partition the graph into **connected components** so that any pair of vertices in the same component is connected, but vertices in different components are not.*



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

Exercise 2

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



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

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

Solution:

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

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

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

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

Useful Facts of Graph Spectrum (Proof of 2)

Let us generalise and formalise the example before!

Proof of 2 (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
   - $\chi_{C_i}^T \mathbf{L} \chi_{C_i} = \frac{1}{d} \cdot \sum_{\{u,v\} \in E} (\chi_{C_i}(u) - \chi_{C_i}(v))^2 = 0 \quad \Rightarrow \quad \lambda_1 = \cdots = \lambda_k = 0$

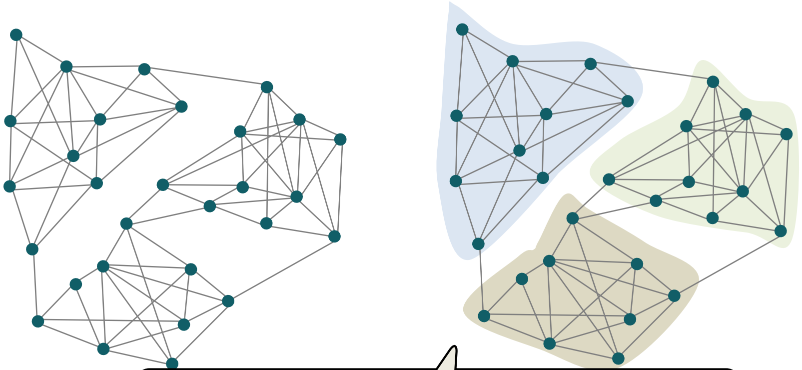
2. ("$\Longleftarrow$" $cc(G) \geq \mathrm{mult}(0)$). We will show:
   $\lambda_1 = \cdots = \lambda_k = 0 \quad \Rightarrow \quad G$ has at least k connected comp. $C_1, \ldots, C_k$
   - there exist $f_1, \ldots, f_k$ orthonormal such that $\sum_{\{u,v\} \in E} (f_i(u) - f_i(v))^2 = 0$
   - $\Rightarrow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

□

Outline

Graph Clustering

*Partition the graph into **pieces (clusters)** so that vertices in the same piece have, on average, more connections among each other than with vertices in other clusters*



Let us for simplicity focus on the case of **two clusters**!

Conductance

Conductance

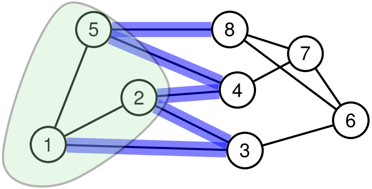
Let $G = (V, E)$ be a d-regular and undirected graph and $\emptyset \neq S \subsetneq V$. The conductance (edge expansion) of S is

$$\phi(S) := \frac{e(S, S^c)}{d \cdot |S|}$$

Moreover, the conductance (edge expansion) of the graph G is

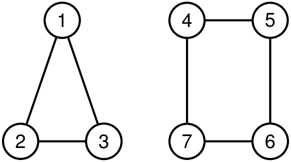
$$\phi(G) := \min_{S \subseteq V:\ 1 \leq |S| \leq n/2} \phi(S)$$

NP-hard to compute!



- $\phi(S) = \frac{5}{9}$
- $\phi(G) \in [0, 1]$ and $\phi(G) = 0$ iff G is disconnected
- If G is a complete graph, then $e(S, V \setminus S) = |S| \cdot (n - |S|)$ and $\phi(G) \approx 1/2$.

λ_2 versus Conductance (1/2)



$$\phi(G) = 0 \quad \Leftrightarrow \quad G \text{ is disconnected} \quad \Leftrightarrow \quad \lambda_2(G) = 0$$

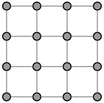
What is the relationship between $\phi(G)$ and $\lambda_2(G)$ for **connected** graphs?

λ_2 versus Conductance (2/2)

1D Grid

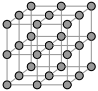
$$\lambda_2 \sim n^{-2}$$
$$\phi \sim n^{-1}$$

2D Grid



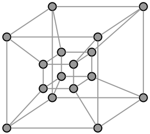
$$\lambda_2 \sim n^{-1}$$
$$\phi \sim n^{-1/2}$$

3D Grid



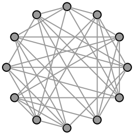
$$\lambda_2 \sim n^{-2/3}$$
$$\phi \sim n^{-1/3}$$

Hypercube



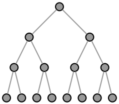
$$\lambda_2 \sim (\log n)^{-1}$$
$$\phi \sim (\log n)^{-1}$$

Random Graph (Expanders)



$$\lambda_2 = \Theta(1)$$
$$\phi = \Theta(1)$$

Binary Tree



$$\lambda_2 \sim n^{-1}$$
$$\phi \sim n^{-1}$$

Relating λ_2 and Conductance

Cheeger's inequality

Let G be a d-regular undirected graph and $\lambda_1 \leq \cdots \leq \lambda_n$ be the eigenvalues of its Laplacian matrix. Then,

$$\frac{\lambda_2}{2} \leq \phi(G) \leq \sqrt{2\lambda_2}.$$

Spectral Clustering:

1. Compute the eigenvector x corresponding to λ_2
2. Order the vertices so that $x_1 \leq x_2 \leq \cdots \leq x_n$ (embed V on $\mathbb{R}$)
3. Try all $n-1$ sweep cuts of the form $(\{1, 2, \ldots, k\}, \{k+1, \ldots, n\})$ and return the one with smallest conductance

- It returns cluster $S \subseteq V$ such that $\phi(S) \leq \sqrt{2\lambda_2} \leq 2\sqrt{\phi(G)}$
- no constant factor worst-case guarantee, but usually works well in practice (see examples later!)
- very fast: can be implemented in $O(|E| \log |E|)$ time

Proof of Cheeger's Inequality (non-examinable)

Proof (of the easy direction):

Optimisation Problem: Embed vertices on a line such that sum of squared distances is minimised

- By the Courant-Fischer Formula,

$$\lambda_2 = \min_{\substack{x \in \mathbb{R}^n \\ x \neq 0, x \perp 1}} \frac{x^T \mathbf{L} x}{x^T x} = \frac{1}{d} \cdot \min_{\substack{x \in \mathbb{R}^n \\ x \neq 0, x \perp 1}} \frac{\sum_{u \sim v} (x_u - x_v)^2}{\sum_u x_u^2}.$$

- Let $S \subseteq V$ be the subset for which $\phi(G)$ is minimised. Define $y \in \mathbb{R}^n$ by:

$$y_u = \begin{cases} \frac{1}{|S|} & \text{if } u \in S, \\ -\frac{1}{|V \setminus S|} & \text{if } u \in V \setminus S. \end{cases}$$

- Since $y \perp 1$, it follows that

$$\lambda_2 \leq \frac{1}{d} \cdot \frac{\sum_{u \sim v} (y_u - y_v)^2}{\sum_u y_u^2} = \frac{1}{d} \cdot \frac{|E(S, V \setminus S)| \cdot (\frac{1}{|S|} + \frac{1}{|V \setminus S|})^2}{\frac{1}{|S|} + \frac{1}{|V \setminus S|}}$$

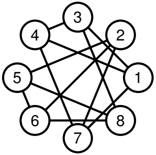
$$= \frac{1}{d} \cdot |E(S, V \setminus S)| \cdot \left(\frac{1}{|S|} + \frac{1}{|V \setminus S|} \right)$$

$$\leq \frac{1}{d} \cdot \frac{2 \cdot |E(S, V \setminus S)|}{|S|} = 2 \cdot \phi(G). \qquad \square$$

Outline

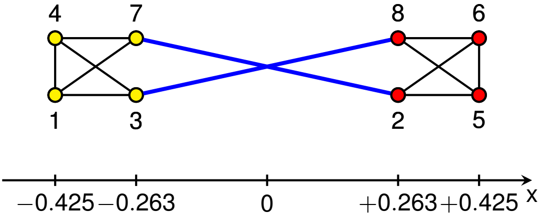
Illustration on a small Example

$$\mathbf{A} = \begin{pmatrix} 0&0&1&1&0&0&1&0\\ 0&0&0&0&1&1&1&0\\ 1&0&0&1&0&0&0&1\\ 1&0&1&0&0&0&1&0\\ 0&1&0&0&0&1&0&1\\ 0&1&0&0&1&0&0&1\\ 1&1&0&1&0&0&0&0\\ 0&0&1&0&1&1&0&0 \end{pmatrix} \quad \mathbf{L} = \begin{pmatrix} 1&0&-\frac{1}{3}&-\frac{1}{3}&0&0&-\frac{1}{3}&0\\ 0&1&0&0&-\frac{1}{3}&-\frac{1}{3}&-\frac{1}{3}&0\\ -\frac{1}{3}&0&1&-\frac{1}{3}&0&0&0&-\frac{1}{3}\\ -\frac{1}{3}&0&-\frac{1}{3}&1&0&0&-\frac{1}{3}&0\\ 0&-\frac{1}{3}&0&0&1&-\frac{1}{3}&0&-\frac{1}{3}\\ 0&-\frac{1}{3}&0&0&-\frac{1}{3}&1&0&-\frac{1}{3}\\ -\frac{1}{3}&-\frac{1}{3}&0&-\frac{1}{3}&0&0&1&0\\ 0&0&-\frac{1}{3}&0&-\frac{1}{3}&-\frac{1}{3}&0&1 \end{pmatrix}$$



$$\lambda_2 = 1 - \sqrt{5}/3 \approx 0.25$$

$$v = (-0.425, +0.263, -0.263, -0.425, +0.425, +0.425, -0.263, +0.263)^T$$



Sweep: 4

Conductance: 0.166

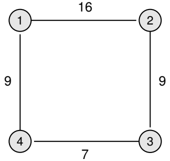
Let us now look at an example of a non-regular graph!

The Laplacian Matrix (General Version)

The (normalised) Laplacian matrix of $G = (V, E, w)$ is the n by n matrix

$$\mathbf{L} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$$

where $\mathbf{D}$ is a diagonal $n \times n$ matrix s.t. $\mathbf{D}_{uu} = deg(u) = \sum_{\{u,v\}\in E} w(u,v)$, and $\mathbf{A}$ is the weighted adjacency matrix of G.



$$\mathbf{L} = \begin{pmatrix} 1 & -16/25 & 0 & -9/20 \\ -16/25 & 1 & -9/20 & 0 \\ 0 & -9/20 & 1 & -7/16 \\ -9/20 & 0 & -7/16 & 1 \end{pmatrix}$$

- $\mathbf{L}_{uv} = \frac{w(u,v)}{\sqrt{d_u d_v}}$ for $u \neq v$
- $\mathbf{L}$ is symmetric
- If G is d-regular, $\mathbf{L} = \mathbf{I} - \frac{1}{d} \cdot \mathbf{A}$.

Conductance and Spectral Clustering (General Version)

Conductance (General Version)

Let $G = (V, E, w)$ and $\emptyset \subsetneq S \subsetneq V$. The conductance (edge expansion) of S is

$$\phi(S) := \frac{w(S, S^c)}{\min\{\mathrm{vol}(S), \mathrm{vol}(S^c)\}},$$

where $w(S, S^c) := \sum_{u \in S, v \in S^c} w(u, v)$ and $\mathrm{vol}(S) := \sum_{u \in S} d(u)$. Moreover, the conductance (edge expansion) of G is

$$\phi(G) := \min_{\emptyset \neq S \subsetneq V} \phi(S).$$

Spectral Clustering (General Version):

1. Compute the eigenvector x corresponding to λ_2 **and** $y = \mathbf{D}^{-1/2} x$.
2. Order the vertices so that $y_1 \leq y_2 \leq \cdots \leq y_n$ (embed V on $\mathbb{R}$)
3. Try all $n - 1$ sweep cuts of the form $(\{1, 2, \ldots, k\}, \{k + 1, \ldots, n\})$ and return the one with smallest conductance

Stochastic Block Model and 1D-Embedding

Stochastic Block Model

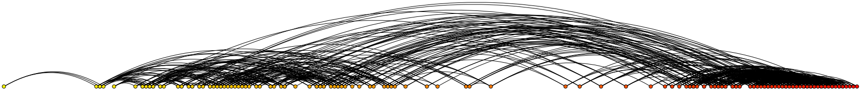
$G = (V, E)$ with clusters $S_1, S_2 \subseteq V$, $0 \leq q < p \leq 1$

$$\mathbf{P}[\{u, v\} \in E] = \begin{cases} p & \text{if } u, v \in S_i, \\ q & \text{if } u \in S_i, v \in S_j, i \neq j. \end{cases}$$

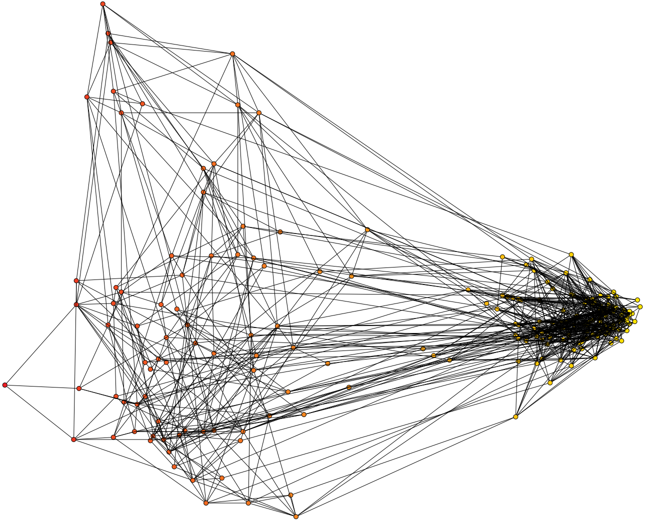
Here:

- $|S_1| = 80$, $|S_2| = 120$
- $p = 0.08$
- $q = 0.01$

```
Number of Vertices: 200
Number of Edges:  919
Eigenvalue  1  :  -1.1968431479565368e-16
Eigenvalue  2  :  0.1543784937248489
Eigenvalue  3  :  0.37049909753568877
Eigenvalue  4  :  0.39770640242147404
Eigenvalue  5  :  0.4316114413430584
Eigenvalue  6  :  0.44379221120189777
Eigenvalue  7  :  0.4564011652684181
Eigenvalue  8  :  0.4632911204500282
Eigenvalue  9  :  0.474638606357877
Eigenvalue  10  :  0.4814019607292904
```



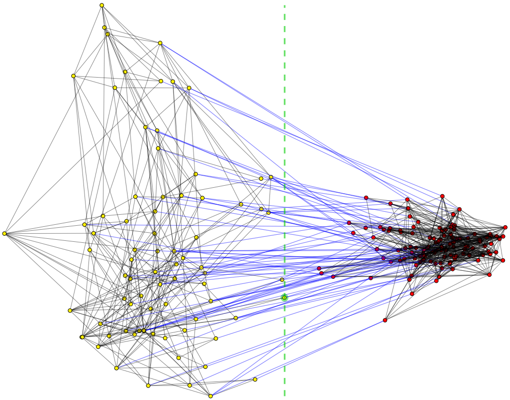
Drawing the 2D-Embedding



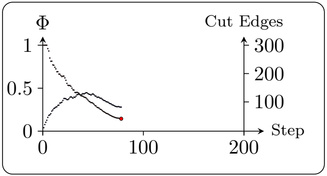
Spectral Clustering

For the animation, see the full slides.

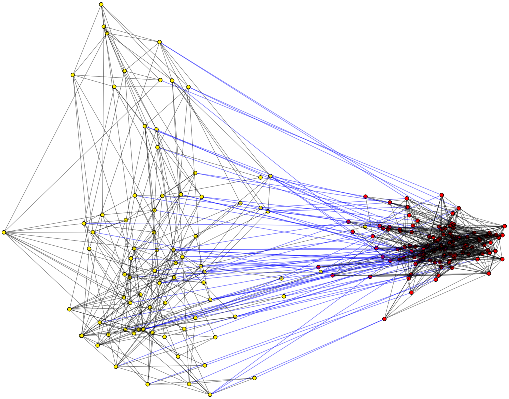
Best Solution found by Spectral Clustering



- Step: 78
- Threshold: −0.0268
- Partition Sizes: 78/122
- Cut Edges: 84
- Conductance: 0.1448



Clustering induced by Blocks



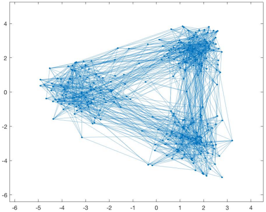
- Step: 1
- Threshold: 0
- Partition Sizes: 80/120
- Cut Edges: 88
- Conductance: 0.1486

Additional Example: Stochastic Block Models with 3 Clusters

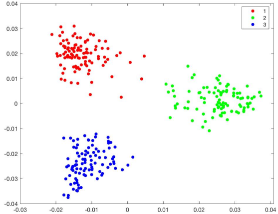
Graph $G = (V, E)$ with clusters
$S_1, S_2, S_3 \subseteq V; \quad 0 \leq q < p \leq 1$

$$\mathbf{P}\left[\{u, v\} \in E\right] = \begin{cases} p & u, v \in S_i \\ q & u \in S_i, v \in S_j, i \neq j \end{cases}$$

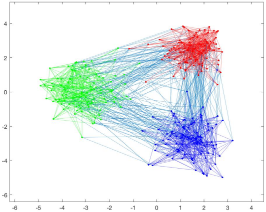
$|V| = 300, |S_i| = 100$
$p = 0.08, q = 0.01.$



Spectral embedding



Output of Spectral Clustering



Choosing the Cluster Number k

- If k is unknown:
  - small λ_k means there exist k sparsely connected subsets in the graph (recall: $\lambda_1 = \ldots = \lambda_k = 0$ means there are k connected components)
  - large λ_{k+1} means all these k subsets have "good" inner-connectivity properties

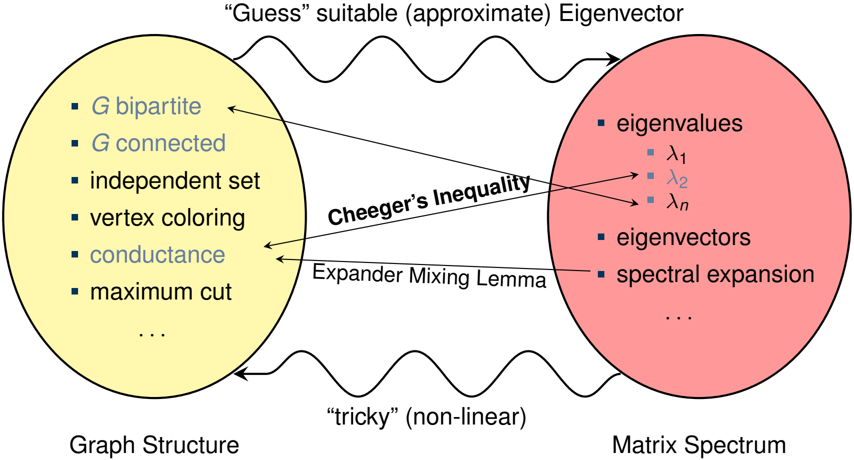
  $\Rightarrow$ choose smallest $k \geq 2$ so that the spectral gap $\lambda_{k+1} - \lambda_k$ is "large"

- In the latter example $\lambda = \{0, 0.20, 0.22, 0.43, 0.45, \ldots\} \implies k = 3.$

- In the former example $\lambda = \{0, 0.15, 0.37, 0.40, 0.43, \ldots\} \implies k = 2.$

- For $k = 2$ use sweep-cut extract clusters. For $k \geq 3$ use embedding in k-dimensional space and apply k-means (geometric clustering)

Summary (1/2): Graph Structure vs. Matrix Spectrum

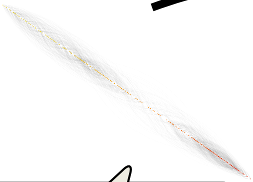


Summary (2/2): Spectral Clustering

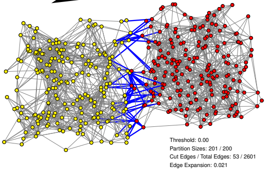
Spectral Embedding onto Line

Compute Sweep Cuts

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



$$\min_{\substack{x \in \mathbb{R}^n \setminus \{\mathbf{0}\} \\ x \perp 1}} \frac{\sum_{u \sim v} (x_u - x_v)^2}{\sum_u x_u^2}$$

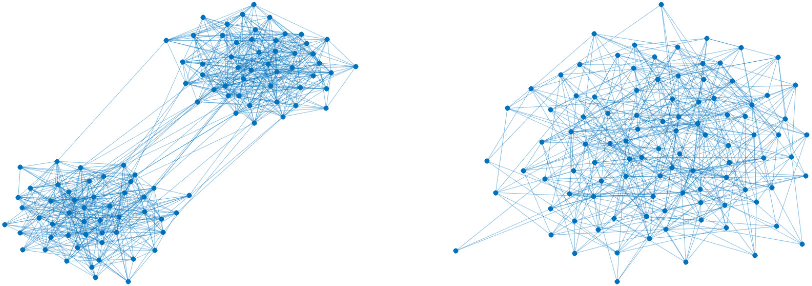


- Given any graph (adjacency matrix)
- Graph Spectrum (computable in poly-time)
  - λ_2 (relates to connectivity)
  - λ_n (relates to bipartiteness)
  - ...
- Cheeger's Inequality
  - relates λ_2 to conductance
  - unbounded approximation ratio
  - effective in practice

Outline

Relation between Clustering and Mixing

- Which graph has a “cluster-structure”?
- Which graph mixes faster?



Convergence of Random Walk

Recall: If the underlying graph G is connected, undirected and d-regular, then the random walk converges towards the stationary distribution $\pi = (1/n, \ldots, 1/n)$, which satisfies $\pi \mathbf{P} = \pi$.

Here all vector multiplications (including eigenvectors) will always be from the left!

Lemma

Consider a lazy random walk on a connected, undirected and d-regular graph. Then for any initial distribution x,

$$\left\| x\mathbf{P}^t - \pi \right\|_2 \leq \lambda^t,$$

with $1 = \lambda_1 > \lambda_2 \geq \cdots \geq \lambda_n$ as eigenvalues and $\lambda := \max\{|\lambda_2|, |\lambda_n|\}$.
$\Rightarrow$ This implies for $t = \mathcal{O}\left(\frac{\log n}{\log(1/\lambda)}\right) = \mathcal{O}\left(\frac{\log n}{1-\lambda}\right)$,

due to laziness, $\lambda_n \geq 0$

$$\left\| x\mathbf{P}^t - \pi \right\|_{tv} \leq \frac{1}{4}.$$

Proof of Lemma

- Express x in terms of the orthonormal basis of $\mathbf{P}$, $v_1 = \pi, v_2, \ldots, v_n$:

$$x = \sum_{i=1}^{n} \alpha_i v_i.$$

- Since x is a probability vector and all $v_i \geq 2$ are orthogonal to π, $\alpha_1 = 1$.

$\Rightarrow$

$$\begin{aligned}
\|x\mathbf{P} - \pi\|_2^2 &= \left\| \left(\sum_{i=1}^{n} \alpha_i v_i \right) \mathbf{P} - \pi \right\|_2^2 \\
&= \left\| \pi + \sum_{i=2}^{n} \alpha_i \lambda_i v_i - \pi \right\|_2^2 \\
&= \left\| \sum_{i=2}^{n} \alpha_i \lambda_i v_i \right\|_2^2 \\
&= \sum_{i=2}^{n} \|\alpha_i \lambda_i v_i\|_2^2 \\
&\leq \lambda^2 \sum_{i=2}^{n} \|\alpha_i v_i\|_2^2 = \lambda^2 \left\| \sum_{i=2}^{n} \alpha_i v_i \right\|_2^2 = \lambda^2 \|x - \pi\|_2^2
\end{aligned}$$

since the v_i's are orthogonal

since the v_i's are orthogonal

- Hence $\|x\mathbf{P}^t - \pi\|_2^2 \leq \lambda^{2t} \cdot \|x - \pi\|_2^2 \leq \lambda^{2t} \cdot 1.$

$\|x - \pi\|_2^2 + \|\pi\|_2^2 = \|x\|_2^2 \leq 1$

Outline

Similarity graph

Given $X = \{x_1, \ldots, x_n\} \in \mathbb{R}^d$, construct $G = (V, E, w)$:

- $x_i \in X \mapsto v_i \in V$
- $E = \binom{V}{2}$
- $w(v_i, v_j) = \exp\left(-\frac{\|x_i - x_j\|^2}{2\sigma^2}\right)$ (Gaussian similarity function)

Remarks:

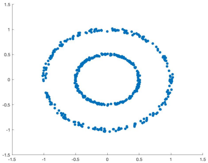
- $w(v_i, v_j)$ is large if x_i is close to x_j
- value of $\sigma \geq 0$ depends on the application (choose it by trial and error, usually $\sigma \in (0.05, 10)$)
- large σ if, on average, pairwise nearest neighbours are far apart

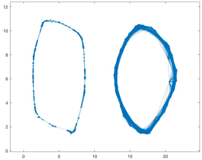
Problem: Since G is complete, from $\Theta(dn)$ to $\Theta(n^2)$ space.

Possible solution: r-nearest neighbour graph ($v_i \sim v_j$ iff x_j is one of the r-nearest neighbours of x_i or vice versa)

From geometric to graph clustering!

Example

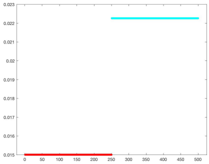




Similarity graph: Gaussian with $\sigma = 0.1$. Only edges with weight ≥ 0.01 shown.

Spectral Clustering (variant for non-regular graphs)

1. Compute the eigenvector x corresponding to λ_2 and $y = \mathbf{D}^{-1/2}x$.
2. Order the vertices so that $y_1 \leq y_2 \leq \cdots \leq y_n$
3. Choose "sweep" cut $(\{1, 2, \ldots, i\}, \{i+1, \ldots, n\})$ with smallest conductance



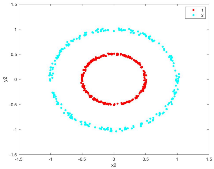


Image segmentation

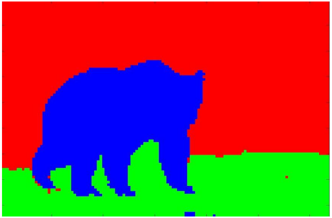
Goal: identify different objects in an image

Construct similarity graph as follows:

- A pixel p is characterised by its position in the image and by its RGB value
- map pixel p in position (x, y) to a vector $v_p = (x, y, r, g, b)$
- construct similarity graph as explained earlier

Original image

Output SC (Gaussian, $\sigma = 10$)



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