

Randomised Algorithms

Lecture 11-12: Spectral Graph Theory and Clustering

Thomas Sauerwald (tms41@cam.ac.uk)

Outline

Introduction to (Spectral) Graph Theory and Clustering

Matrices, Spectrum and Structure

A Simplified Clustering Problem

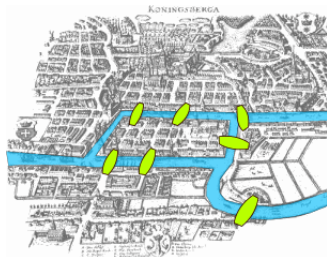
Conductance, Cheeger's Inequality and Spectral Clustering

Illustrations of Spectral Clustering and Extension to Non-Regular Graphs

Relating Spectrum to Mixing Times

Outlook: Glimpse at Image Segmentation (non-examinable)

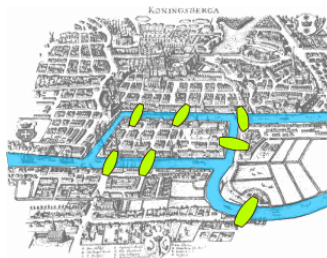
Origin of Graph Theory



Source: Wikipedia

Seven Bridges at Königsberg 1737

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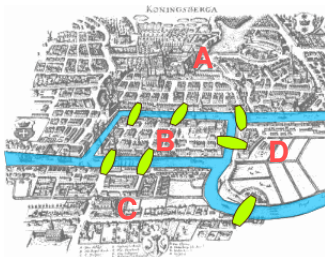


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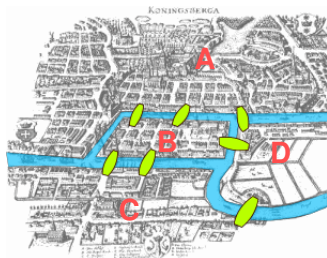


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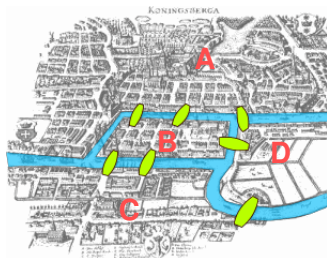


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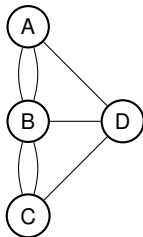
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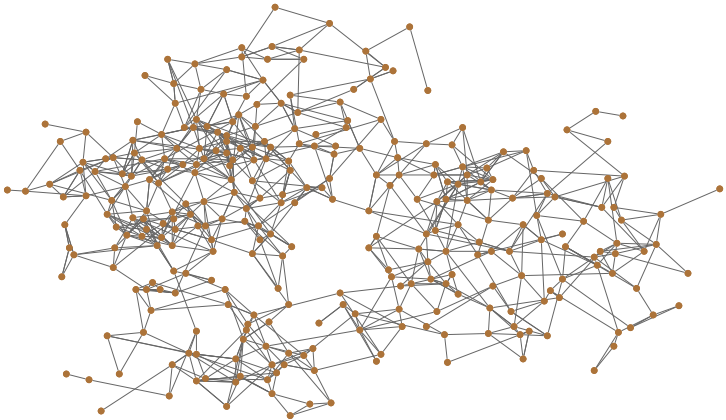
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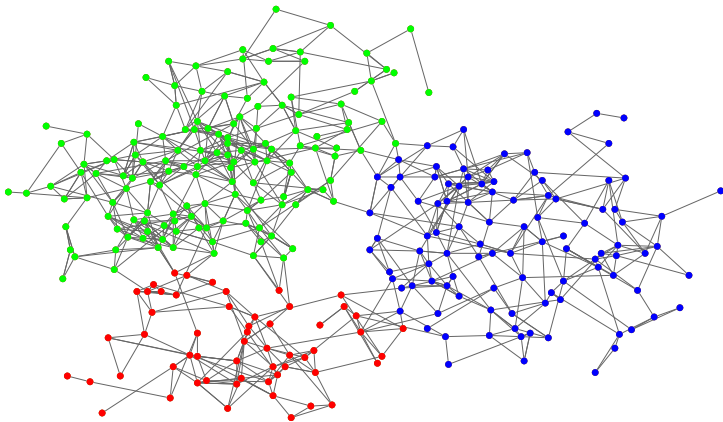


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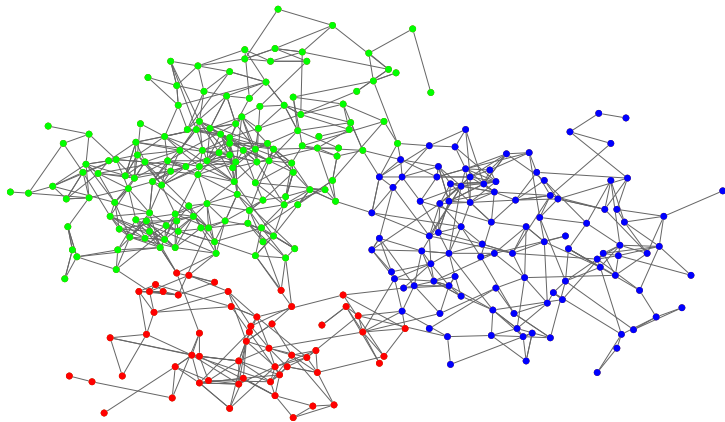
Graphs Nowadays: Clustering



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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
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(there is no ground truth (usually), and we cannot learn from mistakes!)

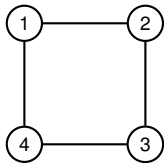
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 - **Graph Clustering**: partition vertices in a graph
 - modularity, conductance, min-cut, etc.

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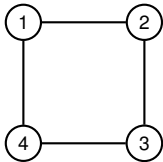
Graphs



Matrices

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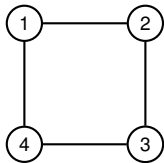
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- Bipartiteness
- Number of triangles
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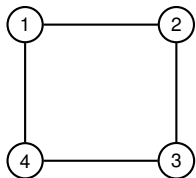
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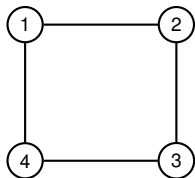
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$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

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 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 .

Eigenvalues and Graph Spectrum of A

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

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

Exercise 1

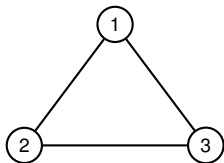


Exercise: What are the Eigenvalues and Eigenvectors?

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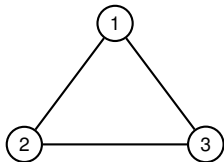
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Bonus: Can you find a short-cut to $\det(\mathbf{A} - \lambda \cdot \mathbf{I})$?



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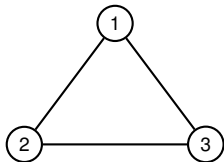
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Solution:

- 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

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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.

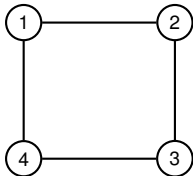
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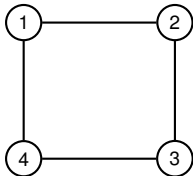
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Correspondence between Adjacency and Laplacian Matrix

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

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

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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.

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

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 $x \in \mathbb{R}^n$,

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

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Proof:

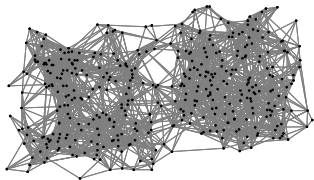
$$\begin{aligned} x^T \mathbf{L} x &= x^T \left(\mathbf{I} - \frac{1}{d} \mathbf{A} \right) x = x^T x - \frac{1}{d} x^T \mathbf{A} x \\ &= \sum_{u \in V} x_u^2 - \frac{2}{d} \sum_{\{u,v\} \in E} x_u x_v \\ &= \frac{1}{d} \sum_{\{u,v\} \in E} (x_u^2 + x_v^2 - 2x_u x_v) \\ &= \sum_{\{u,v\} \in E} \frac{(x_u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

Visualising a Graph

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

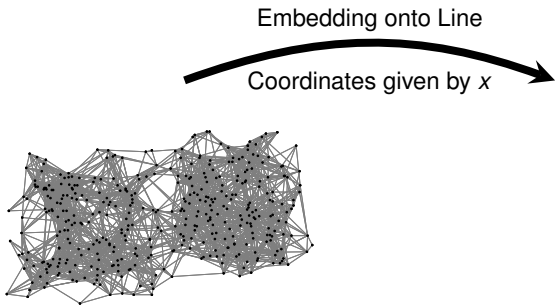
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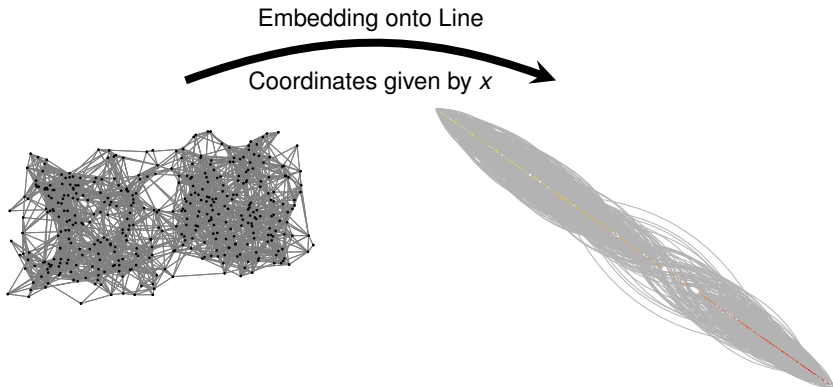
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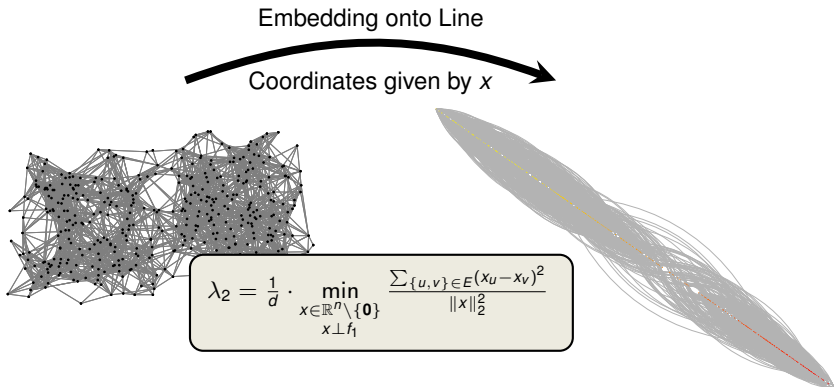
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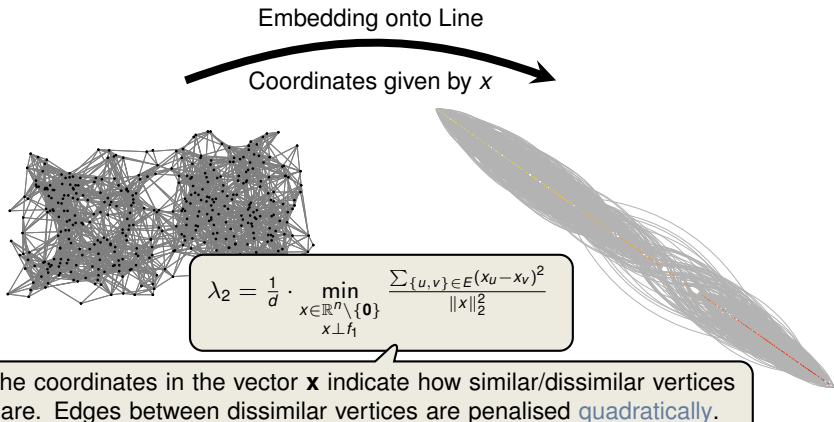
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Outline

Introduction to (Spectral) Graph Theory and Clustering

Matrices, Spectrum and Structure

A Simplified Clustering Problem

Conductance, Cheeger's Inequality and Spectral Clustering

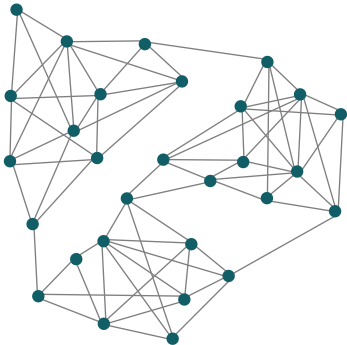
Illustrations of Spectral Clustering and Extension to Non-Regular Graphs

Relating Spectrum to Mixing Times

Outlook: Glimpse at Image Segmentation (non-examinable)

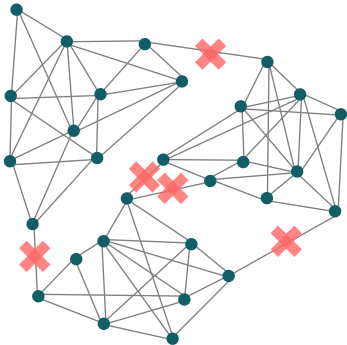
A Simplified Clustering Problem

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.



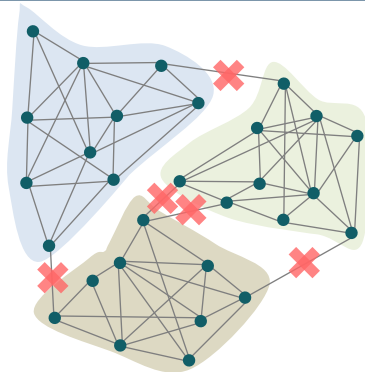
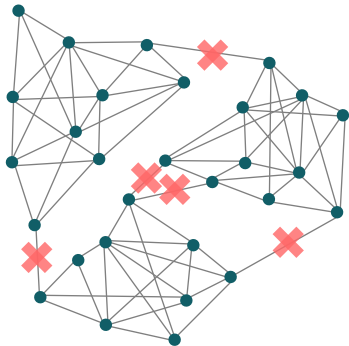
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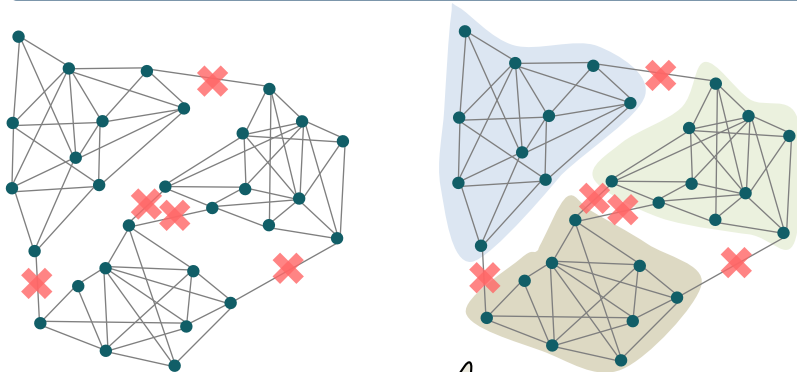
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We could obviously solve this easily using DFS/BFS, but let's see how we can tackle this using the **spectrum of L** !

Exercise 2

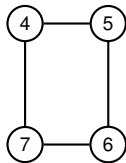
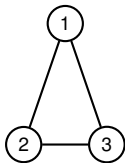


Exercise: What are the Eigenvectors with Eigenvalue 0 of \mathbf{L} ?

Exercise 2



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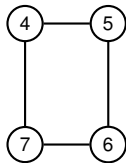
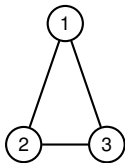


$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \end{pmatrix}$$

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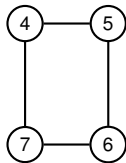
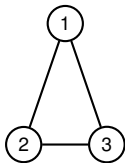
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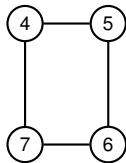
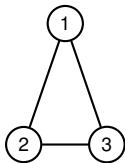
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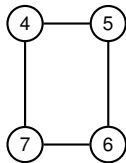
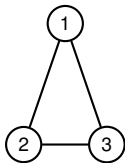
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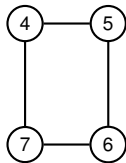
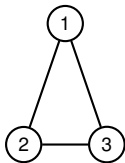
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Next section: A fine-grained approach works even if the clusters are **sparsely** connected!

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- as f_1, \dots, f_k are pairwise orthogonal, G must have k different connected components.

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$\lambda_1 = \dots = \lambda_k = 0 \implies G$ 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.

□

Outline

Introduction to (Spectral) Graph Theory and Clustering

Matrices, Spectrum and Structure

A Simplified Clustering Problem

Conductance, Cheeger's Inequality and Spectral Clustering

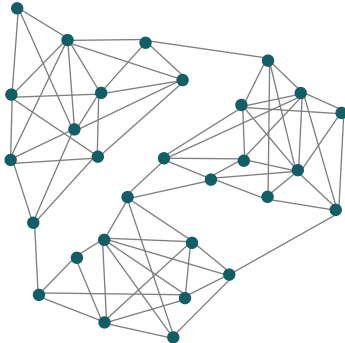
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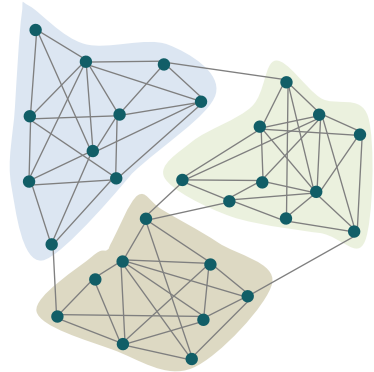
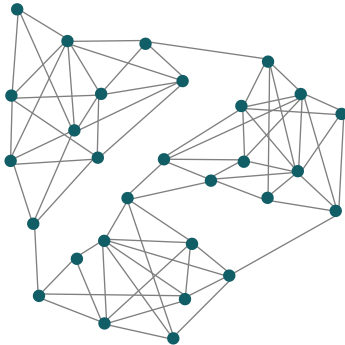
Graph Clustering

*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*



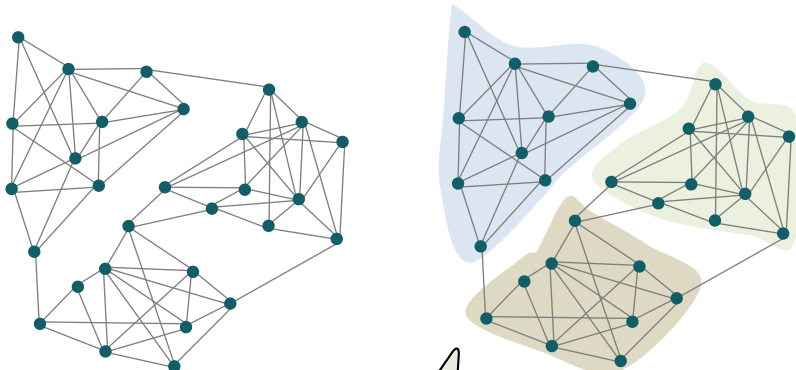
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Let us for simplicity focus on the case of **two clusters**!

Conductance

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

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

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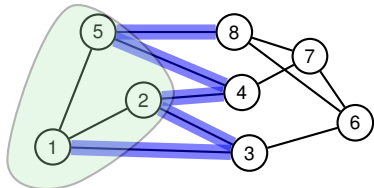
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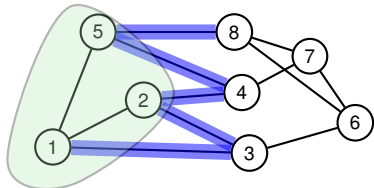
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- $\phi(S) = ??$

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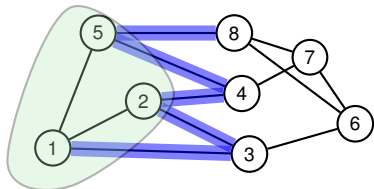
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▪ $\phi(S) = \frac{5}{9}$

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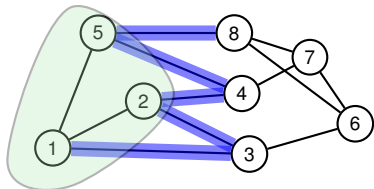
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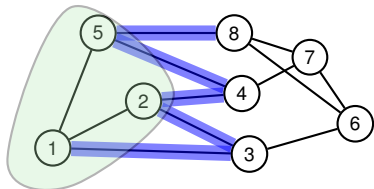
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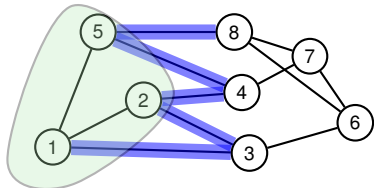
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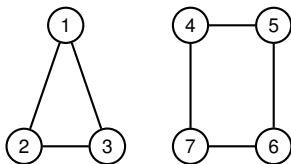
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NP-hard to compute!

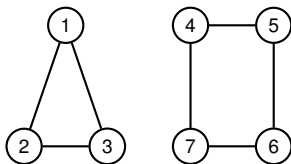


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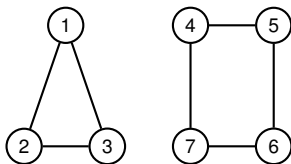
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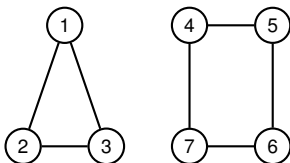
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$\phi(G) = 0 \iff G$ is disconnected



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



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

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

λ_2 versus Conductance (2/2)

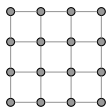
1D Grid



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

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

2D Grid



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3D Grid



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

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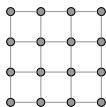
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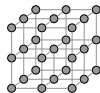
2D Grid



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

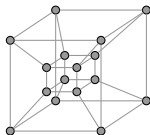
3D Grid



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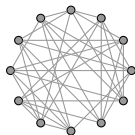
Hypercube



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

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

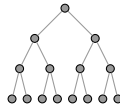
Random Graph (Expanders)



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

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

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 $\lambda_1 \leq \dots \leq \lambda_n$ be the eigenvalues of its Laplacian matrix. Then,

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

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- 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

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

$$\begin{aligned} \lambda_2 &\leq \frac{1}{d} \cdot \frac{\sum_{u \sim v} (y_u - y_v)^2}{\sum_u y_u^2} = \frac{1}{d} \cdot \frac{|E(S, V \setminus S)| \cdot \left(\frac{1}{|S|} + \frac{1}{|V \setminus S|}\right)^2}{\frac{1}{|S|} + \frac{1}{|V \setminus S|}} \\ &= \frac{1}{d} \cdot |E(S, V \setminus S)| \cdot \left(\frac{1}{|S|} + \frac{1}{|V \setminus S|}\right) \\ &\leq \frac{1}{d} \cdot \frac{2 \cdot |E(S, V \setminus S)|}{|S|} = 2 \cdot \phi(G). \quad \square \end{aligned}$$

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Illustration on a small Example

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

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

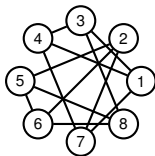
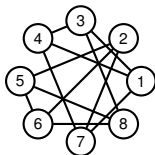


Illustration on a small Example

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

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



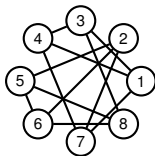
$$\lambda_2 = 1 - \sqrt{5}/3 \approx 0.25$$

$$\mathbf{v} = (-0.425, +0.263, -0.263, -0.425, +0.425, +0.425, -0.263, +0.263)^T$$

Illustration on a small Example

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

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



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

$$\mathbf{v} = (-0.425, +0.263, -0.263, -0.425, +0.425, +0.425, -0.263, +0.263)^T$$

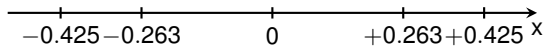
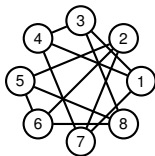


Illustration on a small Example

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

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



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

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

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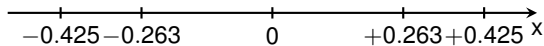
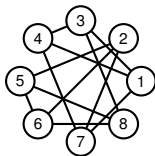


Illustration on a small Example

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

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



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

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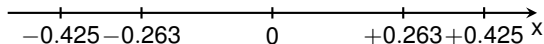
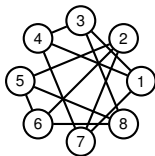


Illustration on a small Example

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

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



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

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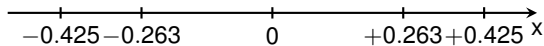
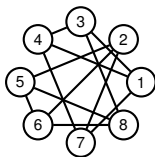


Illustration on a small Example

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

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



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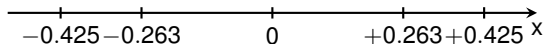
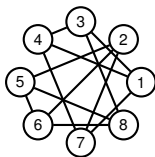


Illustration on a small Example

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

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



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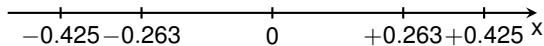
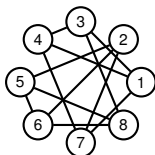


Illustration on a small Example

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

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



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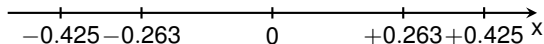
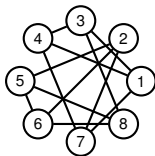
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Illustration on a small Example

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

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



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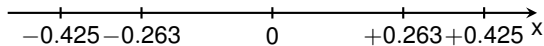
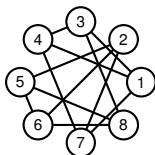


Illustration on a small Example

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

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



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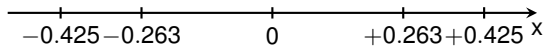
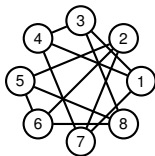


Illustration on a small Example

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

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



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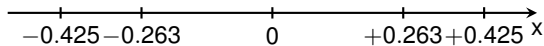
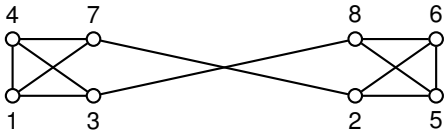
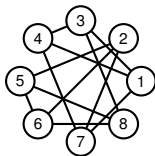


Illustration on a small Example

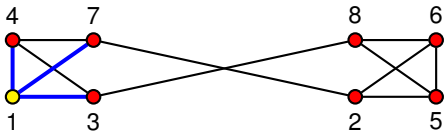
$$A = \begin{pmatrix} 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 \end{pmatrix}$$

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



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Sweep: 1

Conductance: 1

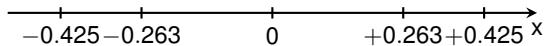
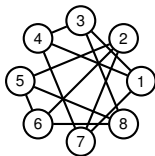


Illustration on a small Example

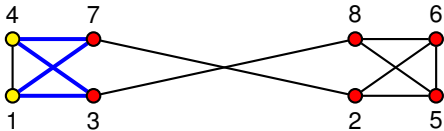
$$A = \begin{pmatrix} 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 \end{pmatrix}$$

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



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

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



Sweep: 2

Conductance: 0.666

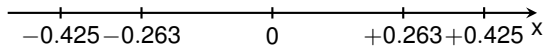
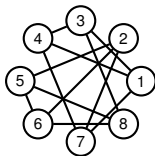


Illustration on a small Example

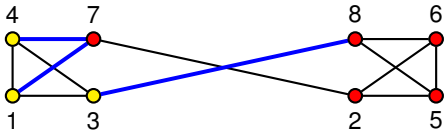
$$A = \begin{pmatrix} 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 \end{pmatrix}$$

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



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

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Sweep: 3

Conductance: 0.333

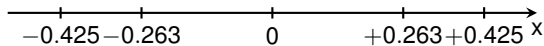
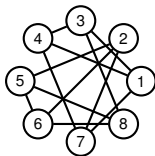


Illustration on a small Example

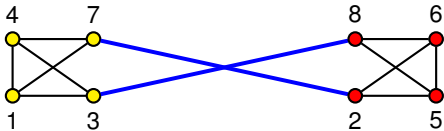
$$A = \begin{pmatrix} 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 \end{pmatrix}$$

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



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

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



Sweep: 4

Conductance: 0.166

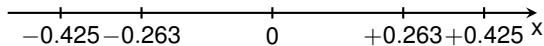
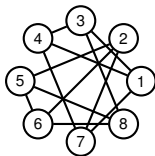


Illustration on a small Example

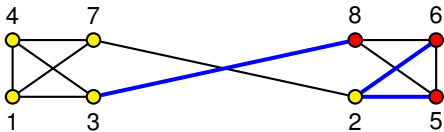
$$A = \begin{pmatrix} 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 \end{pmatrix}$$

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



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

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Sweep: 5

Conductance: 0.333

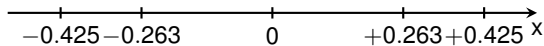
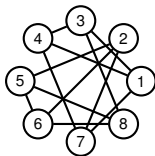


Illustration on a small Example

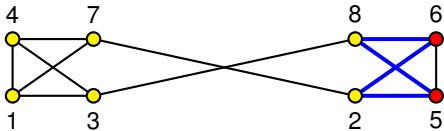
$$A = \begin{pmatrix} 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 \end{pmatrix}$$

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



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Sweep: 6

Conductance: 0.666

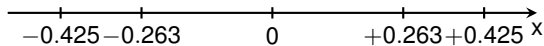
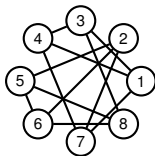


Illustration on a small Example

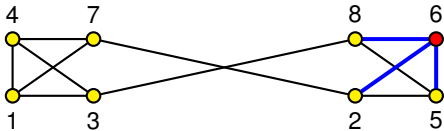
$$A = \begin{pmatrix} 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 \end{pmatrix}$$

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



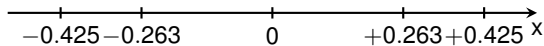
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Sweep: 7

Conductance: 1



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

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

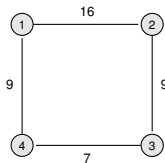
where \mathbf{D} is a diagonal $n \times n$ matrix s.t. $\mathbf{D}_{uu} = \text{deg}(u) = \sum_{\{u,v\} \in E} w(u,v)$, and \mathbf{A} is the weighted adjacency matrix of G .

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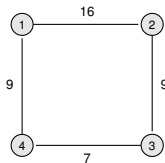
$$\mathbf{L} = \begin{pmatrix} 1 & -16/25 & 0 & -9/20 \\ -16/25 & 1 & -9/20 & 0 \\ 0 & -9/20 & 1 & -7/16 \\ -9/20 & 0 & -7/16 & 1 \end{pmatrix}$$

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- $\mathbf{L}_{uv} = \frac{w(u,v)}{\sqrt{d_u d_v}}$ 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

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

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

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3. Try all $n - 1$ **sweep cuts** of the form $(\{1, 2, \dots, k\}, \{k + 1, \dots, n\})$ and return the one with smallest conductance

Stochastic Block Model and 1D-Embedding

Stochastic Block Model

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

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

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Here:

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

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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

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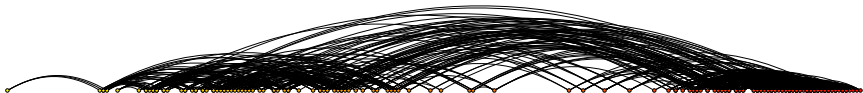
Eigenvalue 6 : 0.44379221120189777

Eigenvalue 7 : 0.4564011652684181

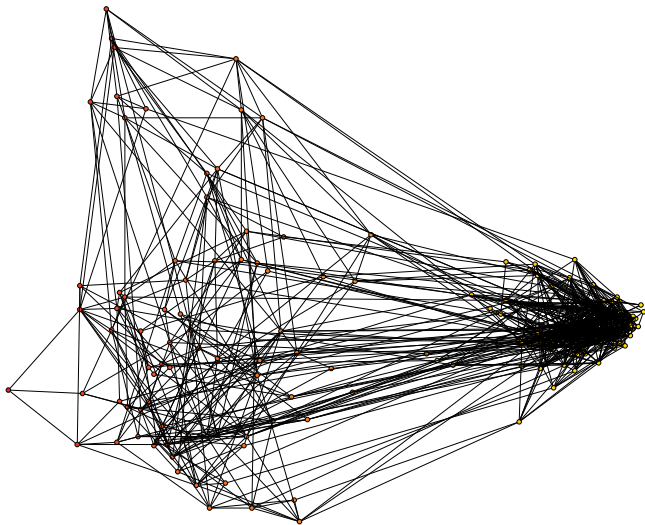
Eigenvalue 8 : 0.4632911204500282

Eigenvalue 9 : 0.474638606357877

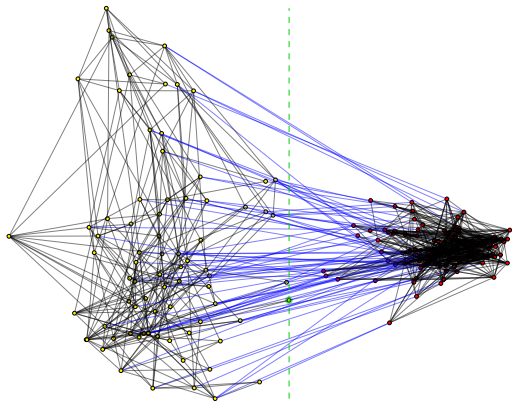
Eigenvalue 10 : 0.4814019607292904



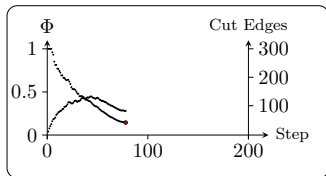
Drawing the 2D-Embedding



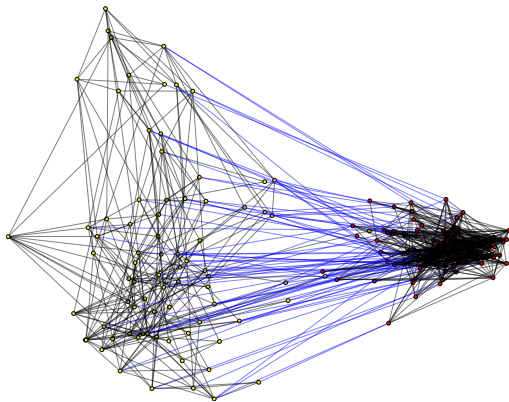
Best Solution found by Spectral Clustering



- 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
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Additional Example: Stochastic Block Models with 3 Clusters

Graph $G = (V, E)$ with clusters

$S_1, S_2, S_3 \subseteq V$; $0 \leq q < p \leq 1$

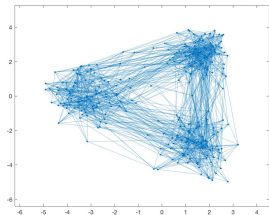
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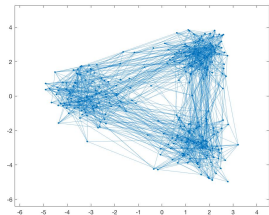


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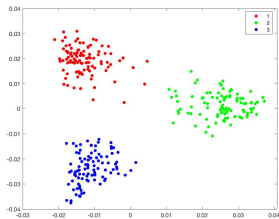
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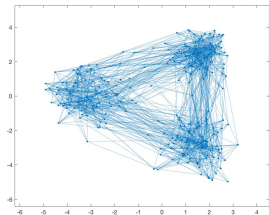


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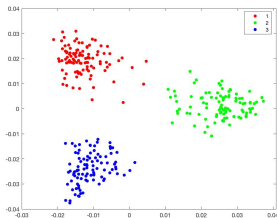
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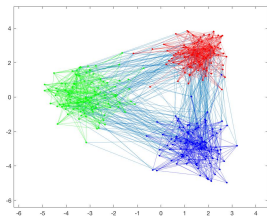
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Spectral embedding



Output of Spectral Clustering



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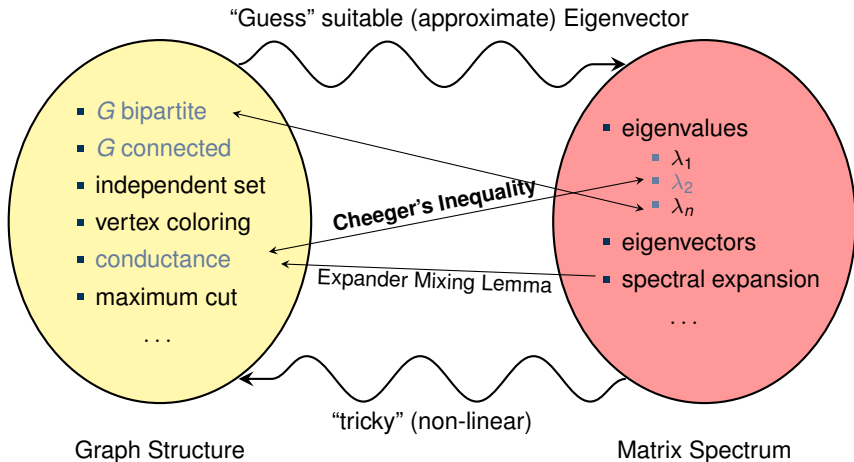
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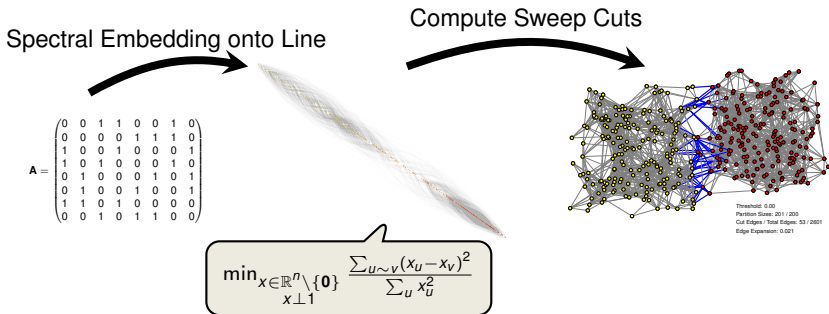
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- For $k = 2$ use sweep-cut extract clusters. For $k \geq 3$ use embedding in k -dimensional space and apply k -means (geometric clustering)

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



Summary (2/2): Spectral Clustering



- 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

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Matrices, Spectrum and Structure

A Simplified Clustering Problem

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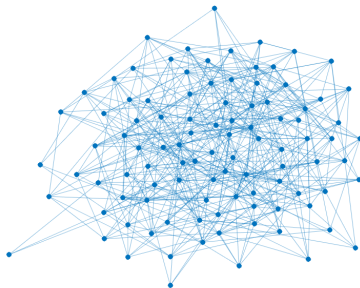
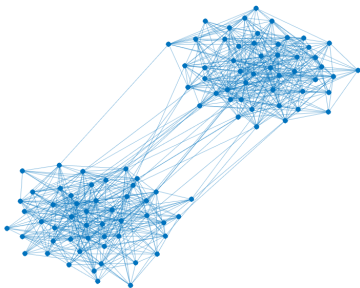
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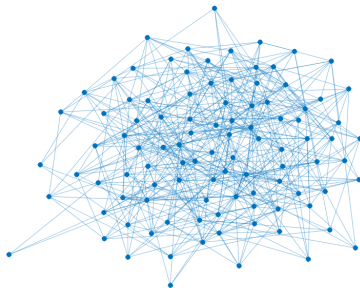
Relation between Clustering and Mixing

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- Which graph has a “cluster-structure”?
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Recall: If the underlying graph G is **connected**, **undirected** and **d -regular**, then the random walk converges towards the **stationary distribution** $\pi = (1/n, \dots, 1/n)$, which satisfies $\pi \mathbf{P} = \pi$.

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\Rightarrow This implies for $t = \mathcal{O}\left(\frac{\log n}{\log(1/\lambda)}\right) = \mathcal{O}\left(\frac{\log n}{1-\lambda}\right)$,

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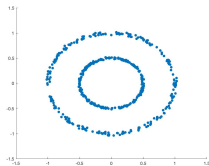
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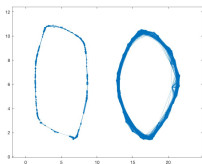
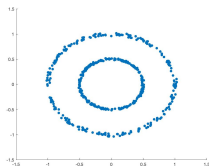
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From geometric to graph clustering!

Example

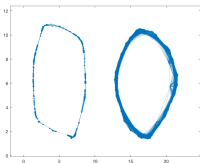
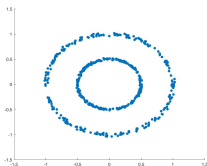


Example



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

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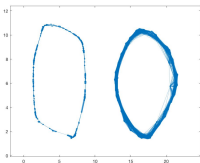
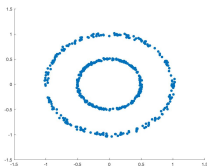


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Spectral Clustering (variant for non-regular graphs)

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

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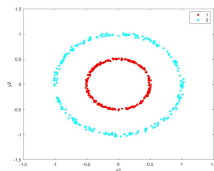
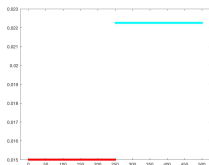


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Original image

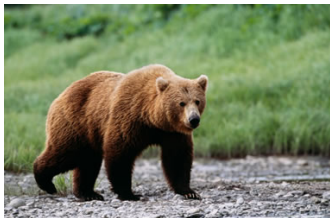


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Output SC (Gaussian, $\sigma = 10$)



References



Fan R.K. Chung.

Graph Theory in the Information Age.

Notices of the AMS, vol. 57, no. 6, pages 726–732, 2010.



Fan R.K. Chung.

Spectral Graph Theory.

Volume 92 of CBMS Regional Conference Series in Mathematics, 1997.



S. Hoory, N. Linial and A. Wigderson.

Expander Graphs and their Applications.

Bulletin of the AMS, vol. 43, no. 4, pages 439–561, 2006.



Daniel Spielman

Chapter 16, Spectral Graph Theory

Combinatorial Scientific Computing



Luca Trevisan.

Lectures Notes on Expansion, Sparsest Cut, and Spectral Graph Theory, 2016.

<https://lucatrevisan.github.io/books/expanders-2016.pdf>