Randomised Algorithms

Lecture 12: Spectral Graph Clustering

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Outline

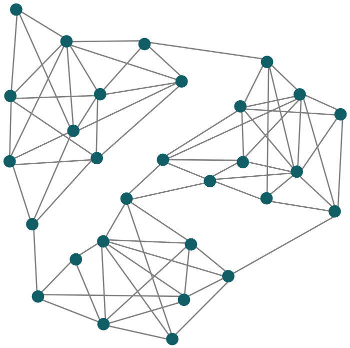
Conductance, Cheeger's Inequality and Spectral Clustering

Illustrations of Spectral Clustering and Extension to Non-Regular Graphs

Appendix: Relating Spectrum to Mixing Times (non-examinable)

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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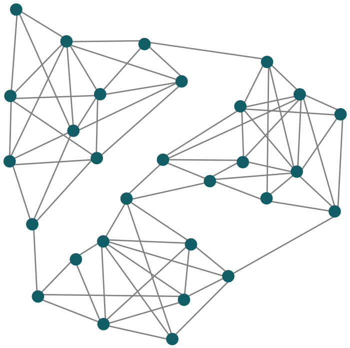

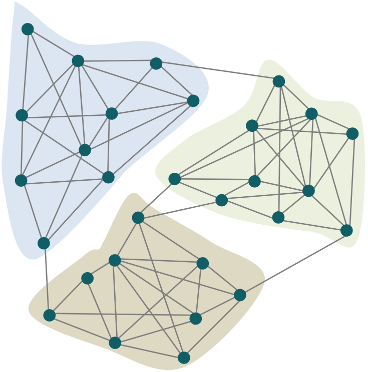

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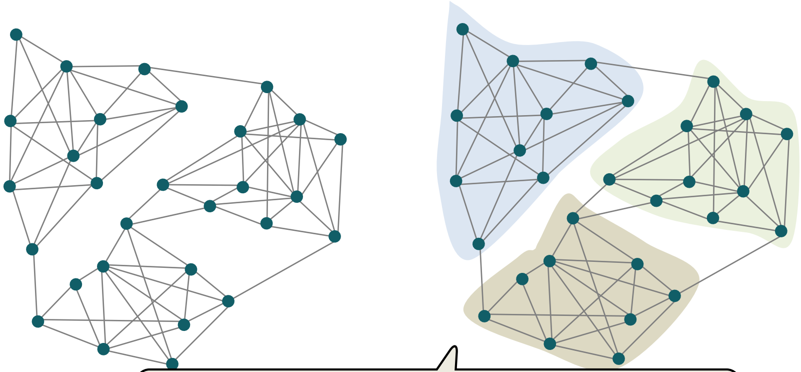

Let us for simplicity focus on the case of **two clusters**!

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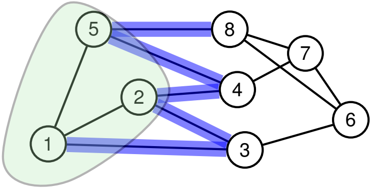

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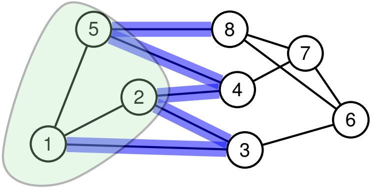

- $\phi(S) = ??$

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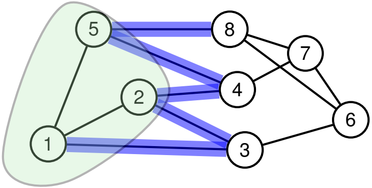

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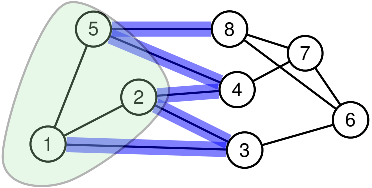

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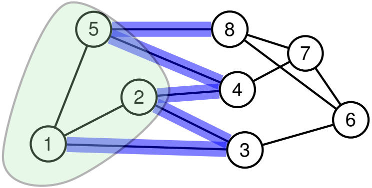

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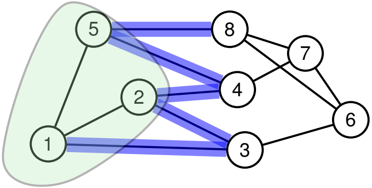
NP-hard to compute!



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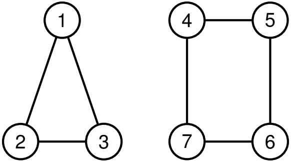

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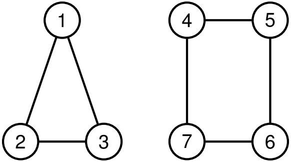

$$\phi(G) = 0 \quad \Leftrightarrow \quad G \text{ is disconnected}$$

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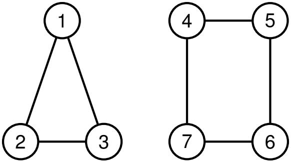

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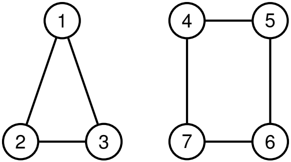

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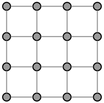
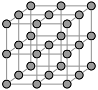
What is the relationship between $\phi(G)$ and $\lambda_2(G)$ for **connected** graphs?

λ_2 versus Conductance (2/2)

1D Grid (Path)	2D Grid	3D Grid
		
$\lambda_2 \sim n^{-2}$	$\lambda_2 \sim n^{-1}$	$\lambda_2 \sim n^{-2/3}$
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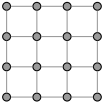

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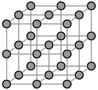
3D Grid



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

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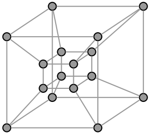
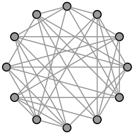
Hypercube



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

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

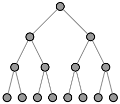
Random Graph (Expanders)



$\lambda_2 = \Theta(1)$

$\phi = \Theta(1)$

Binary Tree



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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,

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

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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

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

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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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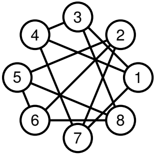
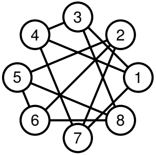


Illustration on a small Example

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

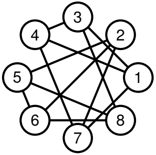


$$\lambda_2 = 1 - \sqrt{5}/3 \approx 0.25$$

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

Illustration on a small Example

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



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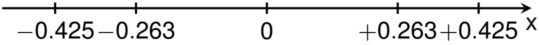

Illustration on a small Example

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

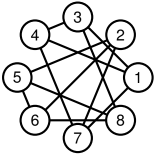

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Illustration on a small Example

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

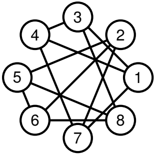

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Illustration on a small Example

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

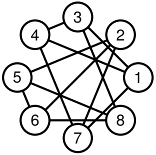

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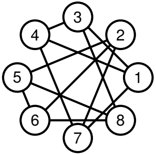
Illustration on a small Example

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



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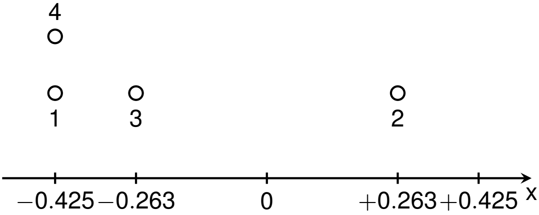
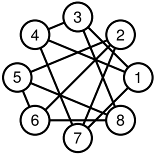


Illustration on a small Example

$$\mathbf{A} = \begin{pmatrix} 0&0&1&1&0&0&1&0\\ 0&0&0&0&1&1&1&0\\ 1&0&0&1&0&0&0&1\\ 1&0&1&0&0&0&1&0\\ 0&1&0&0&0&1&0&1\\ 0&1&0&0&1&0&0&1\\ 1&1&0&1&0&0&0&0\\ 0&0&1&0&1&1&0&0 \end{pmatrix} \qquad \mathbf{L} = \begin{pmatrix} 1&0&-\frac13&-\frac13&0&0&-\frac13&0\\ 0&1&0&0&-\frac13&-\frac13&-\frac13&0\\ -\frac13&0&1&-\frac13&0&0&0&-\frac13\\ -\frac13&0&-\frac13&1&0&0&-\frac13&0\\ 0&-\frac13&0&0&1&-\frac13&0&-\frac13\\ 0&-\frac13&0&0&-\frac13&1&0&-\frac13\\ -\frac13&-\frac13&0&-\frac13&0&0&1&0\\ 0&0&-\frac13&0&-\frac13&-\frac13&0&1 \end{pmatrix}$$



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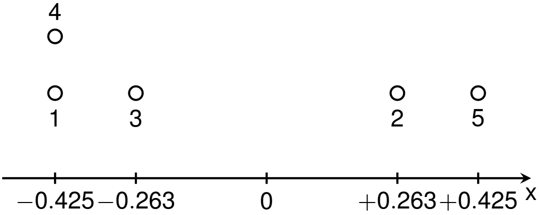
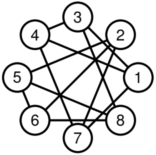


Illustration on a small Example

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



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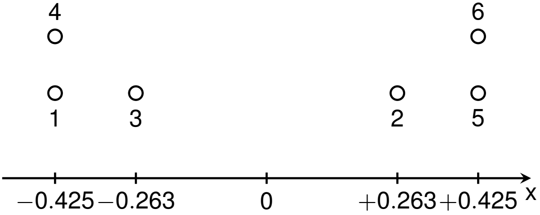
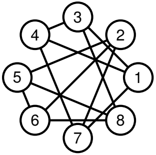


Illustration on a small Example

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



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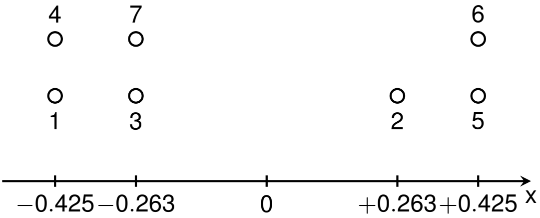
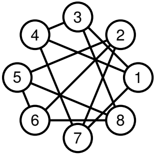


Illustration on a small Example

$$\mathbf{A} = \begin{pmatrix} 0&0&1&1&0&0&1&0\\ 0&0&0&0&1&1&1&0\\ 1&0&0&1&0&0&0&1\\ 1&0&1&0&0&0&1&0\\ 0&1&0&0&0&1&0&1\\ 0&1&0&0&1&0&0&1\\ 1&1&0&1&0&0&0&0\\ 0&0&1&0&1&1&0&0 \end{pmatrix} \qquad \mathbf{L} = \begin{pmatrix} 1&0&-\frac13&-\frac13&0&0&-\frac13&0\\ 0&1&0&0&-\frac13&-\frac13&-\frac13&0\\ -\frac13&0&1&-\frac13&0&0&0&-\frac13\\ -\frac13&0&-\frac13&1&0&0&-\frac13&0\\ 0&-\frac13&0&0&1&-\frac13&0&-\frac13\\ 0&-\frac13&0&0&-\frac13&1&0&-\frac13\\ -\frac13&-\frac13&0&-\frac13&0&0&1&0\\ 0&0&-\frac13&0&-\frac13&-\frac13&0&1 \end{pmatrix}$$



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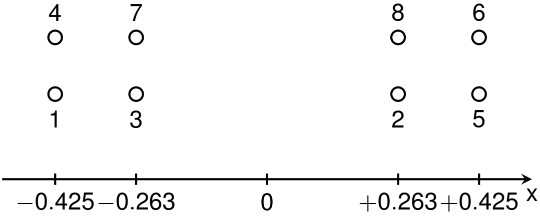
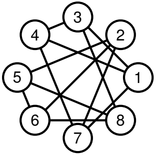


Illustration on a small Example

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



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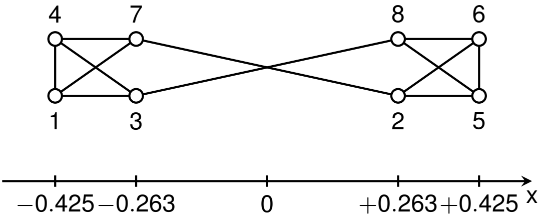
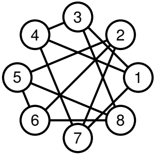


Illustration on a small Example

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



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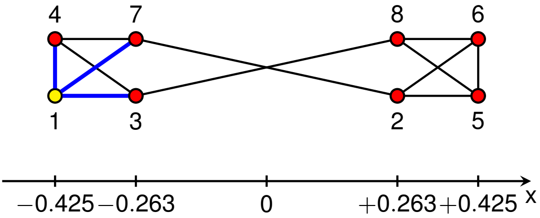
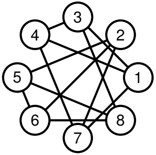


Sweep: 1

Conductance: 1

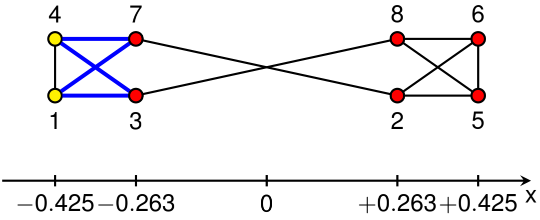
Illustration on a small Example

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



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

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

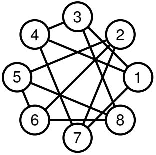


Sweep: 2

Conductance: 0.666

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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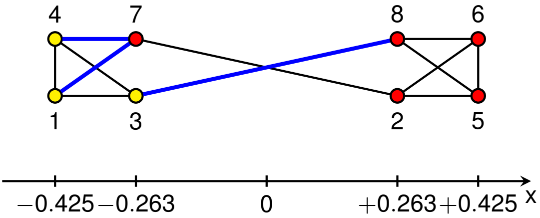
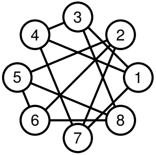


Sweep: 3

Conductance: 0.333

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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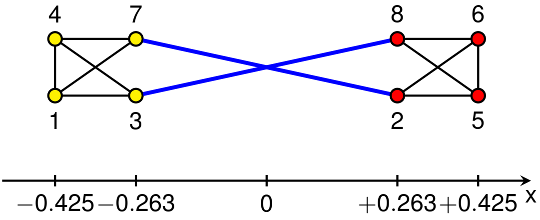
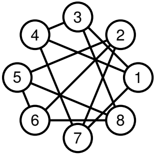


Sweep: 4

Conductance: 0.166

Illustration on a small Example

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



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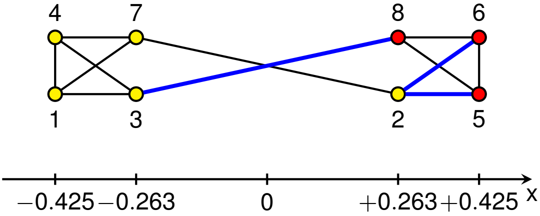
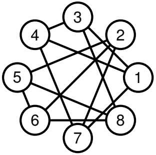


Sweep: 5

Conductance: 0.333

Illustration on a small Example

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



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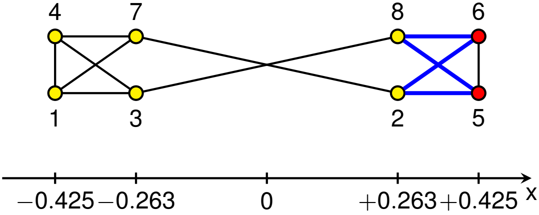

Sweep: 6

Conductance: 0.666

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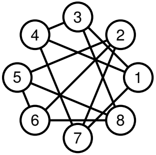

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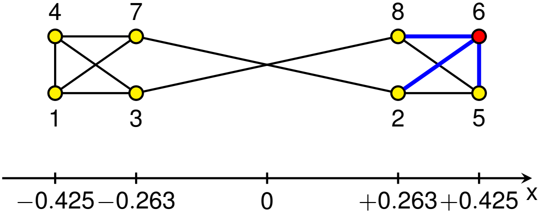

Sweep: 7

Conductance: 1

Physical Interpretation of the Minimisation Problem

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$$\lambda_2 = \min_{\substack{x \in \mathbb{R}^n \setminus \{\mathbf{0}\} \\ x \perp \mathbf{1}}} \frac{x^T \mathbf{L} x}{x^T x}$$

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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 such that $\mathbf{D}_{uu} = \mathtt{deg}(u) = \sum_{v\colon \{u,v\}\in E} w(u,v)$, and $\mathbf{A}$ is the weighted adjacency matrix of G.

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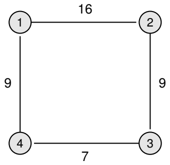

$$\mathbf{L} = \begin{pmatrix} 1 & -16/25 & 0 & -9/20 \\ -16/25 & 1 & -9/20 & 0 \\ 0 & -9/20 & 1 & -7/16 \\ -9/20 & 0 & -7/16 & 1 \end{pmatrix}$$

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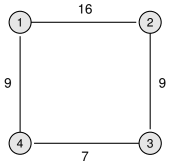

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- $\mathbf{L}_{uv} = -\frac{w(u,v)}{\sqrt{d_u d_v}}$ for $u \neq v$
- $\mathbf{L}$ is symmetric
- If G is d-regular, $\mathbf{L} = \mathbf{I} - \frac{1}{d} \cdot \mathbf{A}$.

Conductance and Spectral Clustering (General Version)

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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

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

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

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Here:

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

Stochastic Block Model and 1D-Embedding

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Here:

- $|S_1| = 80$, $|S_2| = 120$
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Number of Vertices: 200
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Eigenvalue  1  :  -1.1968431479565368e-16
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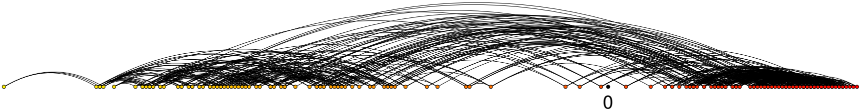
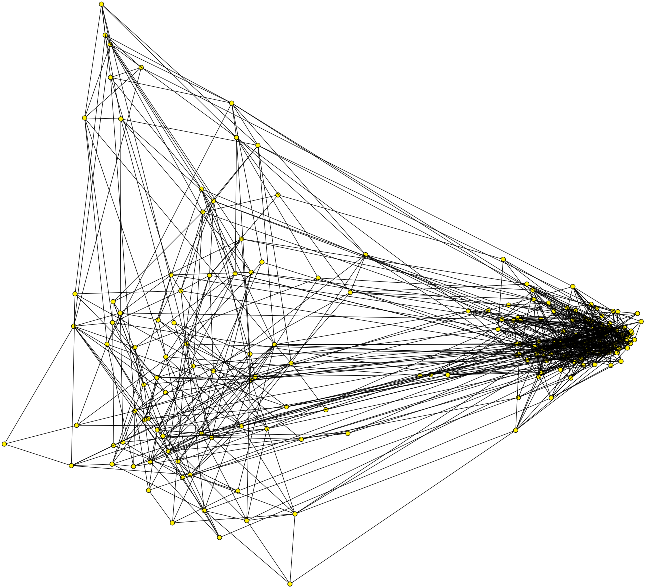
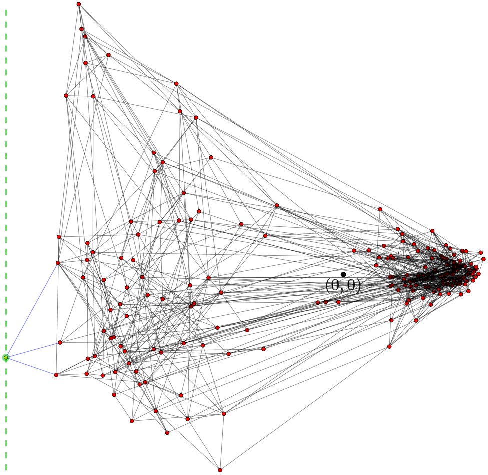


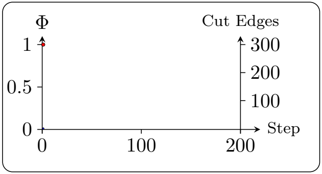
Drawing the 2D-Embedding



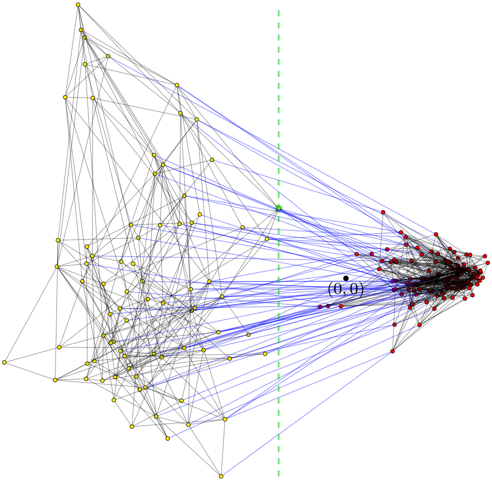
Spectral Clustering



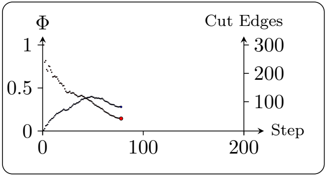
- Step: 1
- Threshold: −0.17
- Partition Sizes: 1/199
- Cut Edges: 3
- Conductance: 1.0



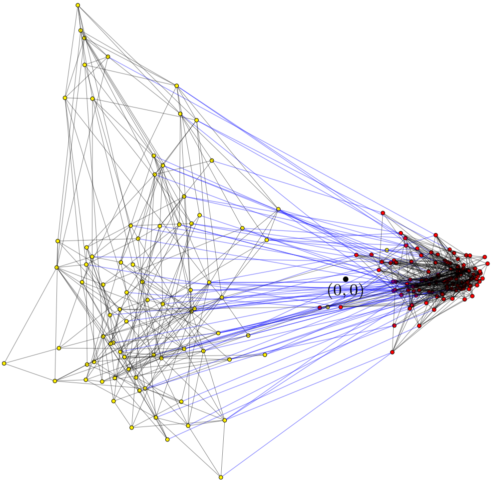
Best Solution found by Spectral Clustering



- Step: 78
- Threshold: -0.0336
- Partition Sizes: 78/122
- Cut Edges: 84
- Conductance: 0.1448



Clustering induced by Blocks



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

Additional Example: Stochastic Block Models with 3 Clusters

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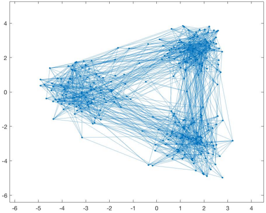

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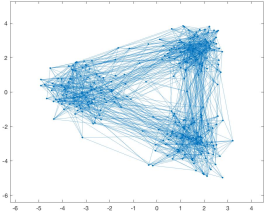
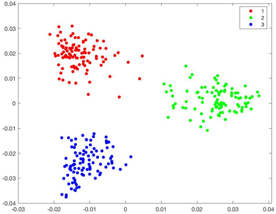


Spectral embedding



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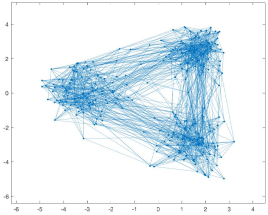

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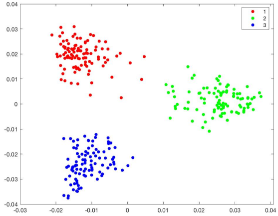
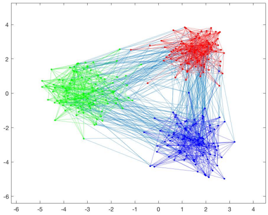


Output of Spectral Clustering



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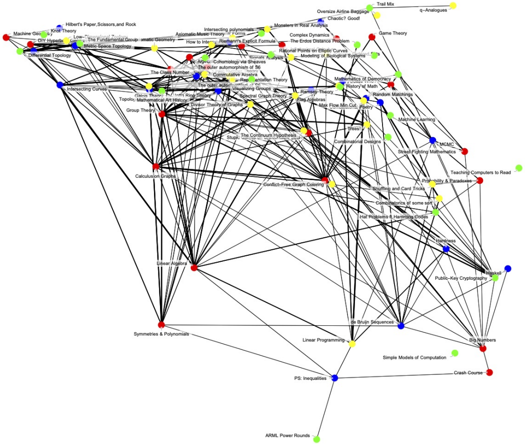
- For $k = 2$ use sweep-cut extract clusters. For $k \geq 3$ use embedding in k-dimensional space and apply k-means (geometric clustering)

Another Example



(many thanks to Kalina Jasinska)

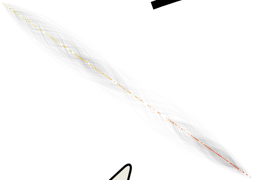
- nodes represent math topics taught within 4 weeks of a Mathcamp
- node colours represent to the week in which they thought
- teachers were asked to assign weights in $0 - 10$ indicating how closely related two classes are

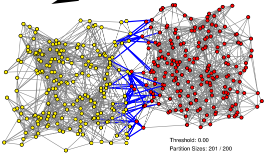
Summary: Spectral Clustering

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

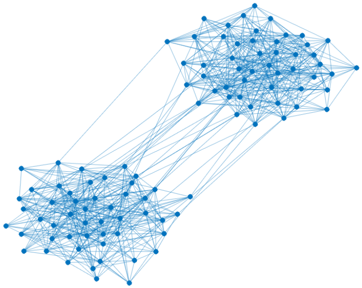
Conductance, Cheeger's Inequality and Spectral Clustering

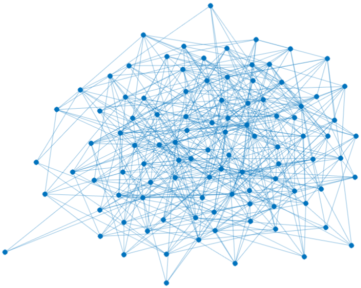
Illustrations of Spectral Clustering and Extension to Non-Regular Graphs

Appendix: Relating Spectrum to Mixing Times (non-examinable)

Relation between Clustering and Mixing (non-examinable)

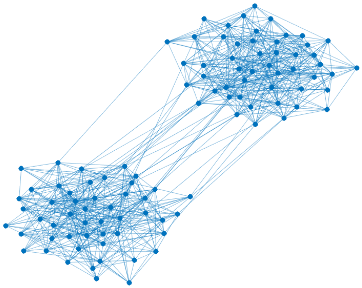
- Which graph has a “cluster-structure”?

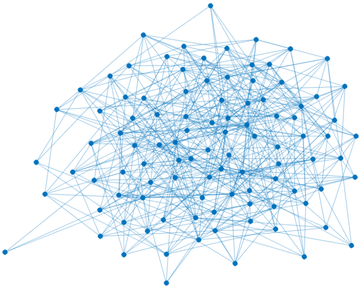




Relation between Clustering and Mixing (non-examinable)

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





Convergence of Random Walk (non-examinable)

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 $\pi \mathbf{P} = \pi$.

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

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

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

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- Hence $\|x\mathbf{P}^t - \pi\|_2^2$

Proof of Lemma (non-examinable)

- 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, $\alpha_1 = 1$.

$\Rightarrow$

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

since the v_i's are orthogonal

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

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\end{aligned}$$

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

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

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The End...

Thank you and Best Wishes for the Exam!

I'm very interested to hear your feedback about the slides and the course more generally. You can use the student feedback form or send me an email during or after the course (`tms41@cam.ac.uk`).