Spectral clustering

He Sun

THE UNIVERSITY of EDINBURGH

Recall: normalised graph Laplacian

Let $G = (V, E, w)$ be an undirected and weighted graph with n vertices and weight function $w : E \to \mathbb{R}_{\geq 0}$. Let $d_u = \sum_{u \sim v} w(u, v)$.

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The normalised Laplacian matrix of G is defined by

$$\mathcal{L} \triangleq \mathbf{I} - \mathbf{D}^{-1/2} \cdot \mathbf{A}\mathbf{D}^{-1/2},$$

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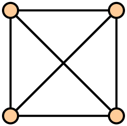

$$\mathcal{L}_G = \begin{pmatrix} 1 & -1/3 & -1/3 & -1/3 \\ -1/3 & 1 & -1/3 & -1/3 \\ -1/3 & -1/3 & 1 & -1/3 \\ -1/3 & -1/3 & -1/3 & 1 \end{pmatrix}$$

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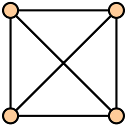

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Matrix $\mathcal{L}$ has eigenvalues $0 = \lambda_1 \leq \ldots \leq \lambda_n$ with corresponding eigenvectors

$$f_1, \ldots, f_n.$$

Recall: graph conductance

The conductance of a set S is defined by

$$\phi_G(S) \triangleq \frac{w(S, V \setminus S)}{\mathrm{vol}(S)},$$

where

$$w(S, V \setminus S) \triangleq \sum_{u \in S, v \in V \setminus S, u \sim v} w(u, v)$$

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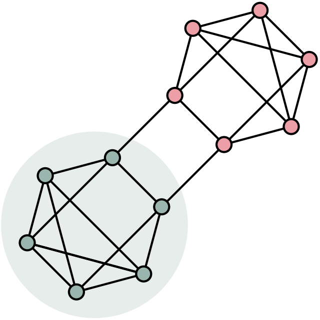

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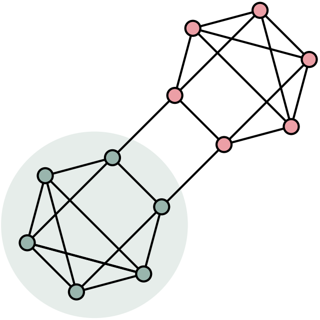

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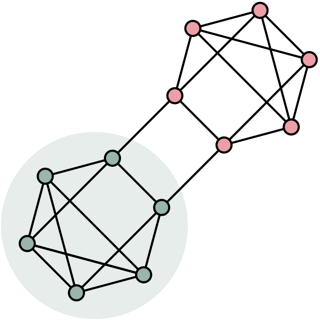

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Cheeger's Inequality

$$\frac{\lambda_2}{2} \leq \phi_G \leq \sqrt{2\lambda_2}.$$

Illustration of the graph partitioning algorithm

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

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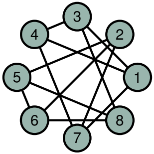

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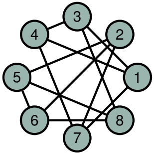

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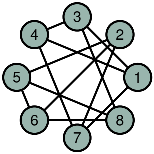

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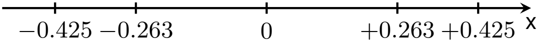

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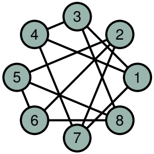

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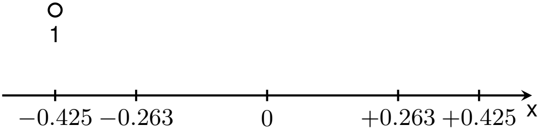

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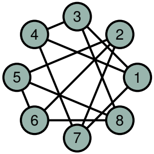

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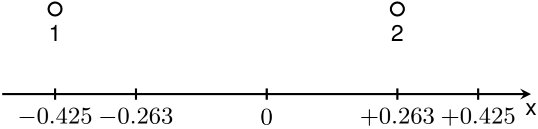

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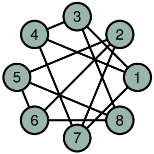

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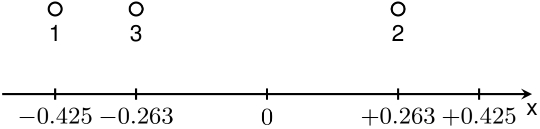

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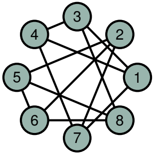

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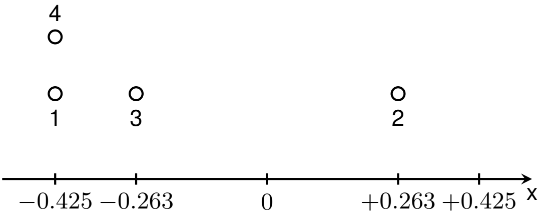

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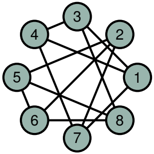

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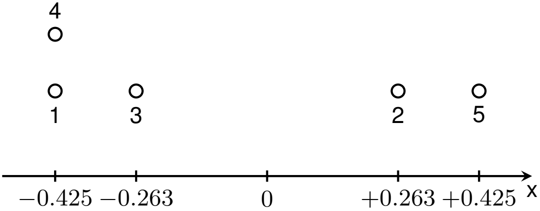
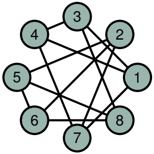


Illustration of the graph partitioning algorithm

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



$$\lambda_2=\sqrt{5}/3\approx 0.75$$

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

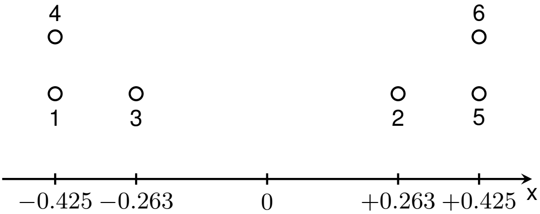
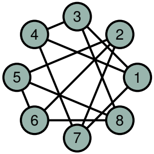


Illustration of the graph partitioning algorithm

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



$$\lambda_2 = \sqrt{5}/3 \approx 0.75$$

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

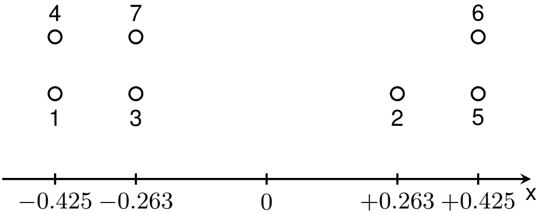
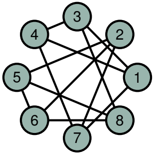


Illustration of the graph partitioning algorithm

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



$$\lambda_2 = \sqrt{5}/3 \approx 0.75$$

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

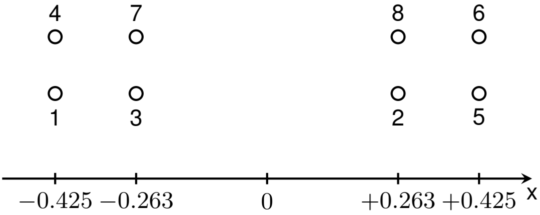
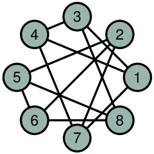


Illustration of the graph partitioning algorithm

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



$$\lambda_2=\sqrt{5}/3\approx 0.75$$

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

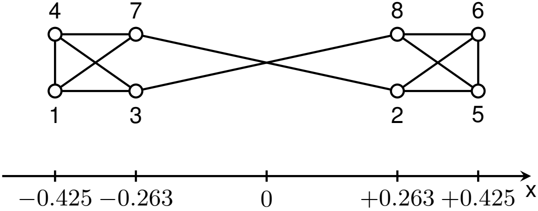
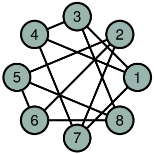


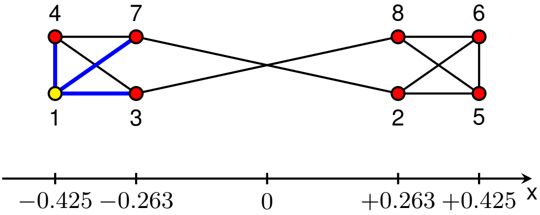
Illustration of the graph partitioning algorithm

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



$$\lambda_2 = \sqrt{5}/3 \approx 0.75$$

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

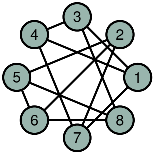


Sweep: 1

Conductance: 1

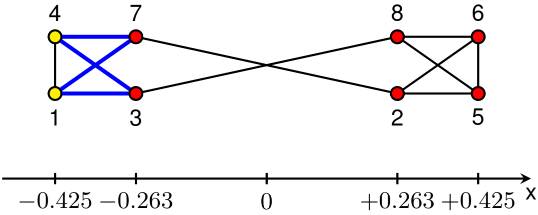
Illustration of the graph partitioning algorithm

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



$$\lambda_2 = \sqrt{5}/3 \approx 0.75$$

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

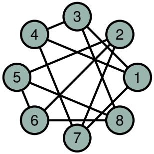


Sweep: 2

Conductance: 0.666

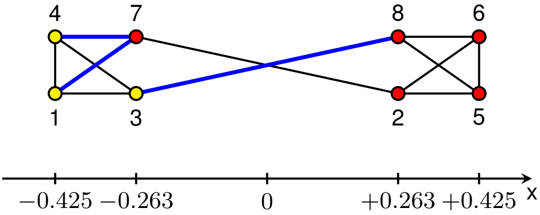
Illustration of the graph partitioning algorithm

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



$$\lambda_2 = \sqrt{5}/3 \approx 0.75$$

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

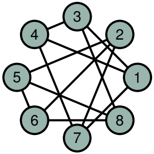


Sweep: 3

Conductance: 0.333

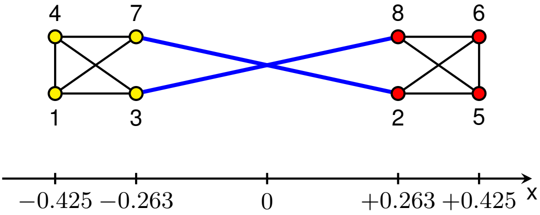
Illustration of the graph partitioning algorithm

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



$$\lambda_2 = \sqrt{5}/3 \approx 0.75$$

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

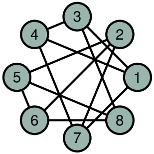


Sweep: 4

Conductance: 0.166

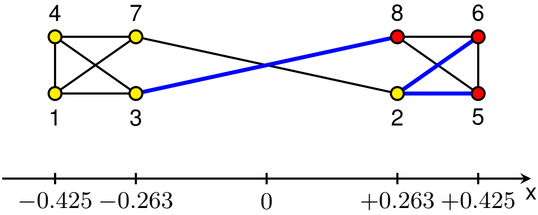
Illustration of the graph partitioning algorithm

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



$$\lambda_2 = \sqrt{5}/3 \approx 0.75$$

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

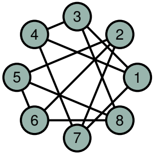


Sweep: 5

Conductance: 0.333

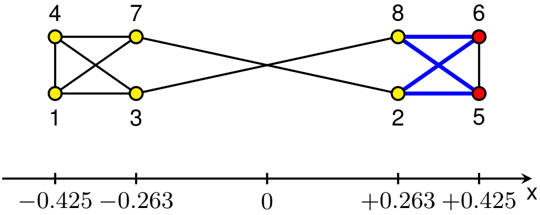
Illustration of the graph partitioning algorithm

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



$$\lambda_2 = \sqrt{5}/3 \approx 0.75$$

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

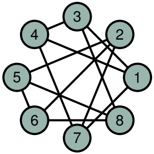


Sweep: 6

Conductance: 0.666

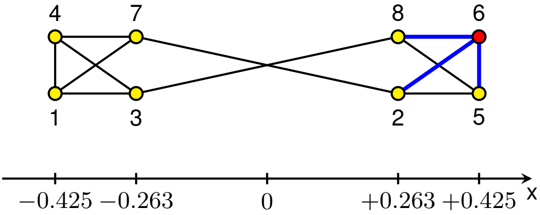
Illustration of the graph partitioning algorithm

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



$$\lambda_2 = \sqrt{5}/3 \approx 0.75$$

$$v = (-0.425, +0.263, -0.263, -0.425, +0.425, +0.425, -0.263, +0.263)^\intercal$$



Sweep: 7

Conductance: 1

Illustration of the graph partition on a large graph

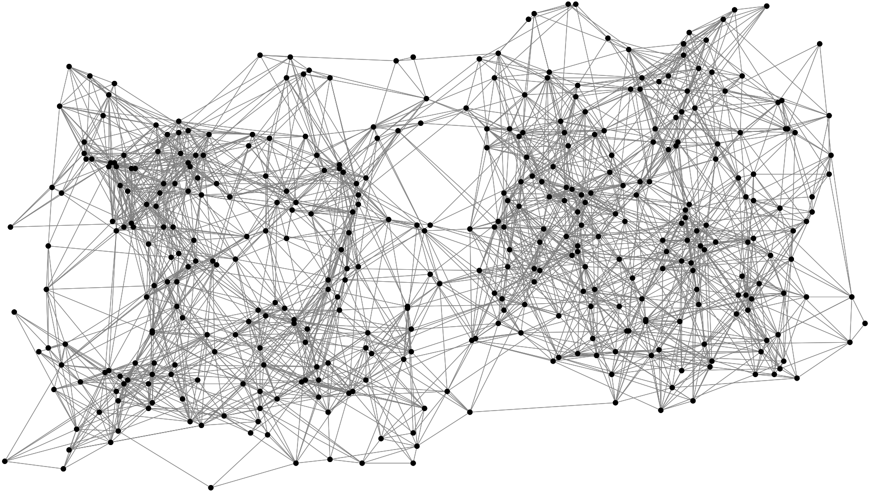


Illustration continues: the second eigenvector

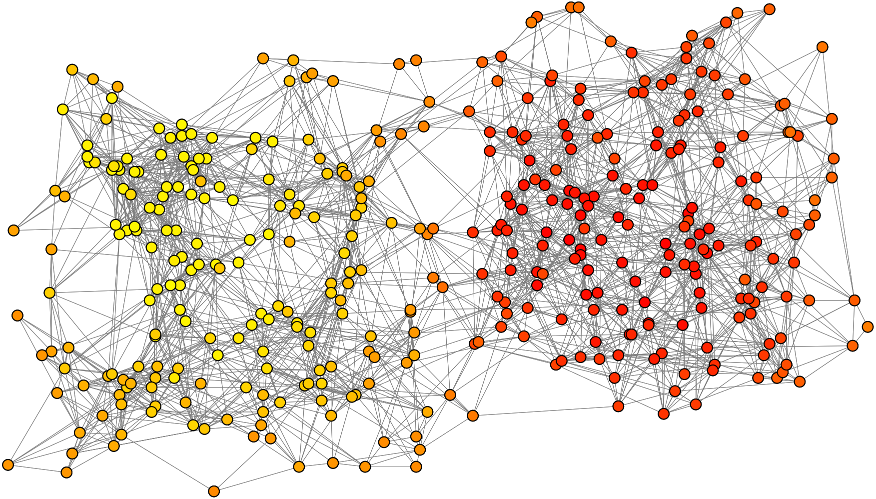
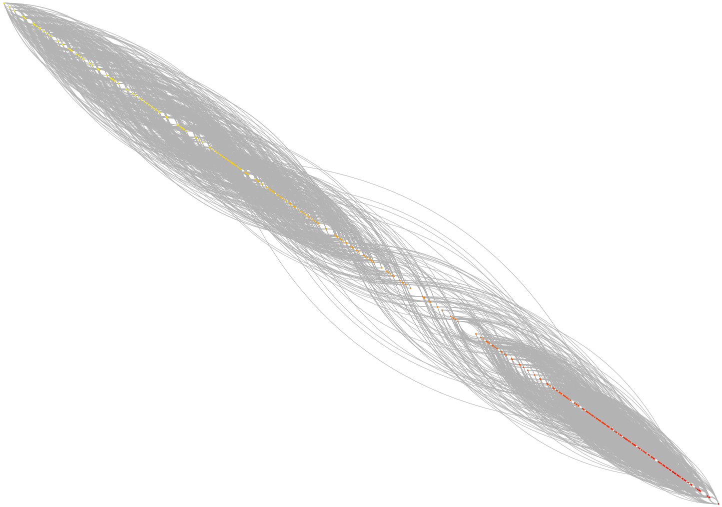
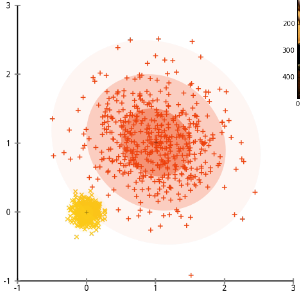


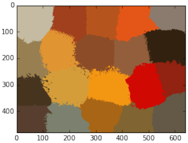
Illustration continues: vertices and edges after the embedding

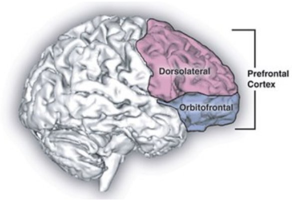


From graph partitioning to graph clustering

Clustering is the task of dividing objects in groups (clusters) so that similar objects are grouped together and dissimilar objects are separated in different groups.



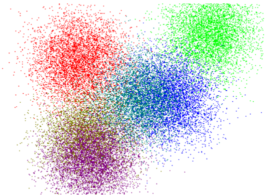




Numerous applications in image segmentation, community detection, bioinformatics, network analysis, among many others

On the hardness of clustering

- One basic learning task in machine learning
  - For many applications training sets are unavailable
- The problem is inherently difficult to be formalised
  - There's no "ground truth"
  - A cluster structure can be defined in many different ways
  - "Impossibility theorem for clustering" (Kleinberg, NIPS '13)
- Most formalisations are actually NP-hard



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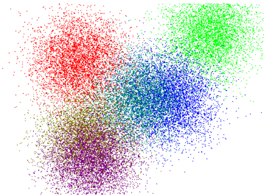
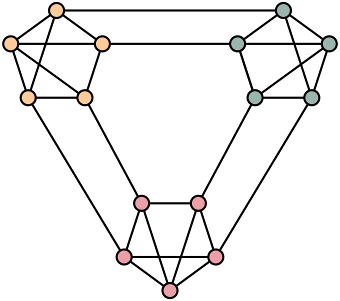


However,

- We have algorithms that "work in practice"
- The more well-clustered the data, the better the quality of the clustering produced

Graph clustering

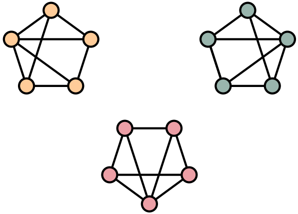
Partition the graph into clusters so that vertices in the same cluster have, on average, more connections among each other than with vertices in other clusters.



Graph clustering via eigenvectors

Lemma (Problem 1 of Homework 5)

Graph G has exactly k connected components iff $\lambda_k = 0$ and $\lambda_{k+1} > 0$.



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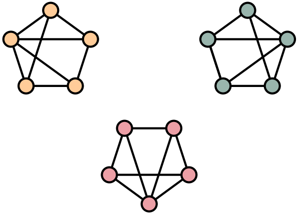

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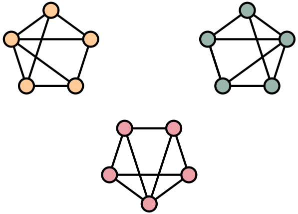
$$\chi_i(v) = \begin{cases} \sqrt{d_v} & \text{if } v \in S_i, \\ 0 & \text{otherwise.} \end{cases}$$



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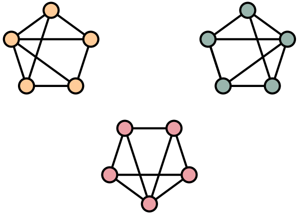

It holds that $\{f_1, \ldots, f_k\} = \{\chi_1, \ldots, \chi_k\}$, i.e., the k eigenvectors can be applied to find k connected components.

Graph clustering via eigenvectors

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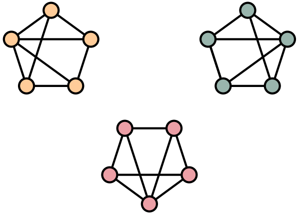

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This situation can be informally viewed as, if $\lambda_k / \lambda_{k+1} = 0$, the structure of k clusters is completed encoded in the bottom k eigenvectors.

Graph clustering via eigenvectors (cont.)

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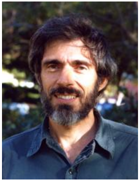
Davis-Kahan Theorem (1970, very informal statement in our setting)

As long as not too many edges between different clusters are added, the k eigenvectors do not change too much.



Chandler Davis

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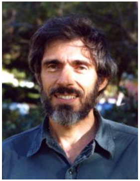

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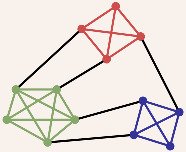
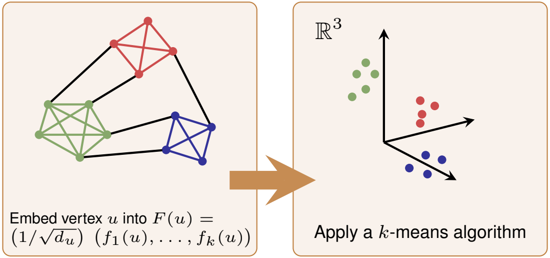
As long as λ_k/λ_{k+1} is small, the k eigenvectors can be used to find k clusters.

Spectral clustering



Embed vertex u into $F(u) = \left(1/\sqrt{d_u}\right) \left(f_1(u), \ldots, f_k(u)\right)$

Spectral clustering



k-means clustering

- Input: Set of n points $x_1, \ldots, x_n$, where $x_i \in \mathbb{R}^d$, and parameter k.
- Goal: Assign the n points to k clusters such that total distance $\sum_{i=1}^{k} \sum_{x \in S_i} \|x - c_i\|^2$ is minimised, where c_i is the centre of cluster S_i.

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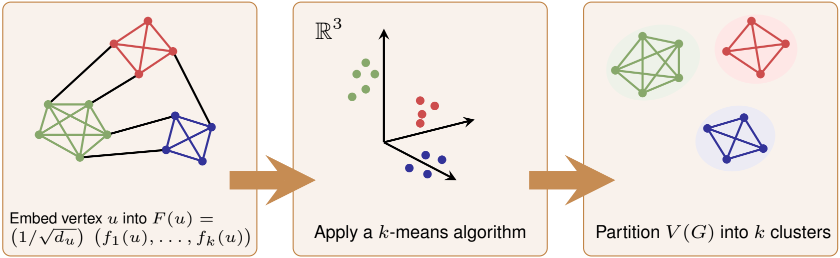

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Practical consideration: choosing the right value of k

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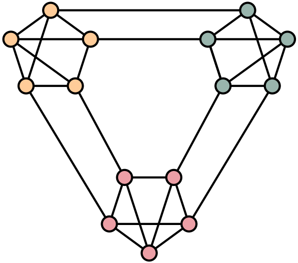
$$\rho(k) = \min_{\text{partition } A_1,\ldots,A_k} \max_{1\leq i\leq k} \phi_G(A_i).$$



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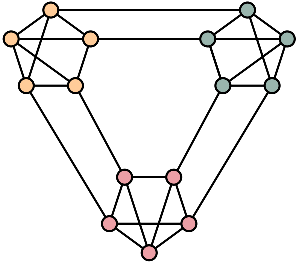

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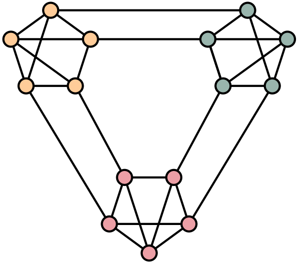

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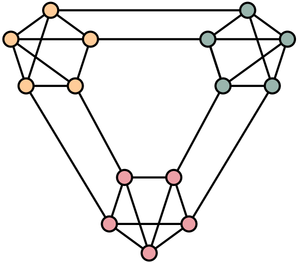

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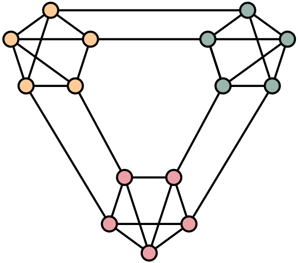

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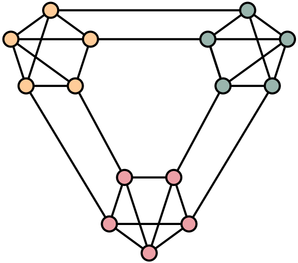

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Example: Assume the eigenvalues are $0,\ 0.20, 0.22,\ 0.5,\ 0.55, \ldots$, then $k = 3$.

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Construction of a similarity graph

Given the set X of points $x_1, \ldots, x_n$, where $x_i \in \mathbb{R}^d$, the similarity graph $G = (V, E, w)$ of X is constructed as follows:

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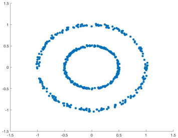
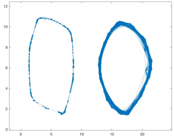
Example: Set $\sigma = 0.1$, and only edges with weight ≥ 0.01 shown.

original graph



similarity graph



Application of spectral clustering in image segmentation

- Every pixel p is characterised by its position in the image and its RGB value, hence every pixel p corresponds to $x_p = (x, y, r, g, b)$.
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Original image

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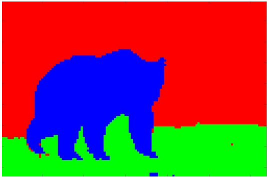
Output ($\sigma = 10$)



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