Spectral Clustering: Theory and Practice

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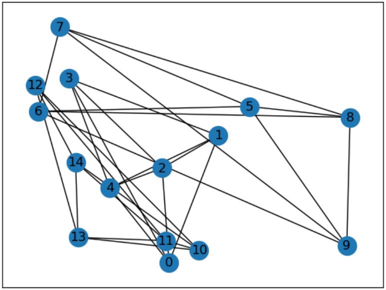
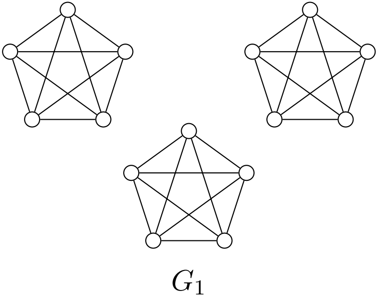
How to find the components?





☺ Breadth-first search ☺ Laplacian matrix

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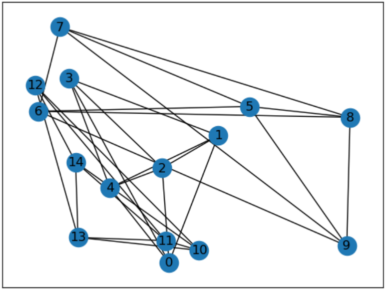
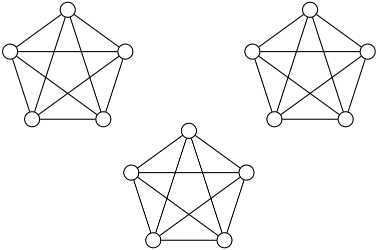
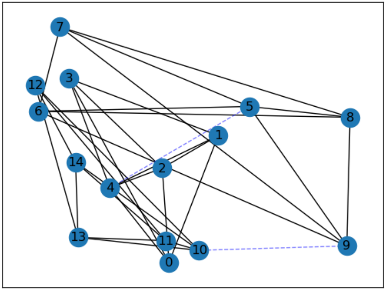


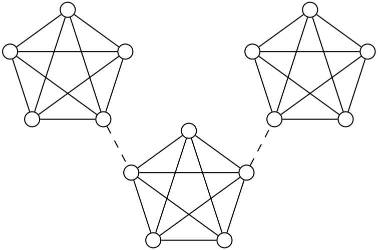


G_1

☺ Breadth-first search ☺ Laplacian matrix

How to find the clusters?

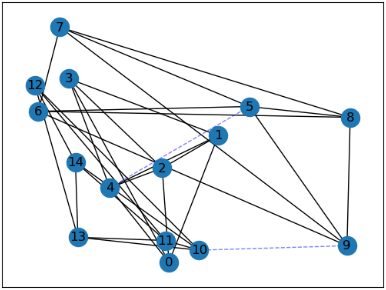


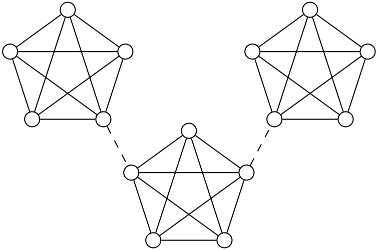


G_2

☹ Breadth-first search ☺ Laplacian matrix

How to find the clusters?





G_2

☹ Breadth-first search ☺ Laplacian matrix

Miroslav Fiedler
1926–2015

Known for

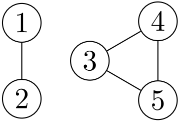
- algebraic connectivity,
- Fiedler vector,
- and more.

Have impact on

- graph partition,
- spectral clustering,
- image segmentation,
- and more.

Source: MacTutor https://mathshistory.st-andrews.ac.uk/Biographies/Fiedler/

Laplacian matrix



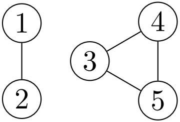
$$\begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 2 & -1 & -1 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & -1 & 2 \end{bmatrix}$$

Definition

Let G be a graph on n vertices. The Laplacian matrix of G is the $n \times n$ matrix $L(G) = \begin{bmatrix} \ell_{i,j} \end{bmatrix}$ such that

$$\ell_{i,j} = \begin{cases} -1 & \text{if } \{i,j\} \in E(G), \\ \deg_G(i) & \text{if } i = j, \\ 0 & \text{otherwise.} \end{cases}$$

Laplacian matrix



$$\begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 2 & -1 & -1 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & -1 & 2 \end{bmatrix}$$

Proposition

1. $L\mathbf{1} = \mathbf{0}$.
2. $\mathbf{x}^\top L\mathbf{x} = \sum_{\{i,j\}\in E}(x_i - x_j)^2$, *which means L is PSD.*
3. $L\mathbf{x} = \mathbf{0} \iff \mathbf{x}^\top L\mathbf{x} = 0$.

Example

For $G = K_2 \dot\cup K_3$,

$$\mathbf{x}^\top L\mathbf{x} = (x_1 - x_2)^2 + (x_3 - x_4)^2 + (x_4 - x_5)^2 + (x_3 - x_5)^2.$$

Count the number of components by the Laplacian matrix

Theorem (Fiedler 1973, Anderson and Morley 1971)

Let G be a graph and $L = L(G)$. Then $\mathrm{null}(L)$ is the number of components of G, and

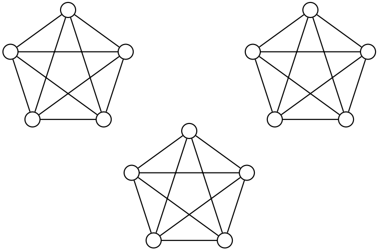
$$\ker(L) = \mathrm{span}\{\phi_{X_1}, \ldots, \phi_{X_k}\},$$

where $X_1, \ldots, X_k$ are the vertex sets of the components of G.

Example

For $G = K_2 \dot\cup K_3$,

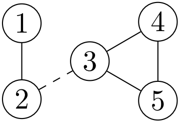
$$\mathrm{spec}(L) = \{0, 0, 2, 3, 3\} \text{ and } \ker(L) = \mathrm{span}\left\{\begin{bmatrix}1\\1\\0\\0\\0\end{bmatrix}, \begin{bmatrix}0\\0\\1\\1\\1\end{bmatrix}\right\}.$$



G_1

$$\mathrm{spec}(L) = \{0, 0, 0, 5, \ldots\} \text{ and } \ker(L) = \mathrm{span}\left\{ \begin{bmatrix} \mathbf{1}_5 \\ \mathbf{0}_5 \\ \mathbf{0}_5 \end{bmatrix}, \begin{bmatrix} \mathbf{0}_5 \\ \mathbf{1}_5 \\ \mathbf{0}_5 \end{bmatrix}, \begin{bmatrix} \mathbf{0}_5 \\ \mathbf{0}_5 \\ \mathbf{1}_5 \end{bmatrix} \right\}.$$

Weighted Laplacian matrix



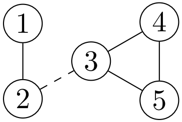
$$\begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 1.1 & -0.1 & 0 & 0 \\ 0 & -0.1 & 2.1 & -1 & -1 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & -1 & 2 \end{bmatrix}$$

Definition

Let G be a weighted graph on n vertices with weights $w_{i,j}$. The weighted Laplacian matrix of G is the $n \times n$ matrix $L(G) = [\ell_{i,j}]$ such that

$$\ell_{i,j} = \begin{cases} -w_{i,j} & \text{if } \{i,j\} \in E(G), \\ \sum_{k:k\sim i} w_{i,k} & \text{if } i = j, \\ 0 & \text{otherwise.} \end{cases}$$

Weighted Laplacian matrix



$$\begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 1.1 & -0.1 & 0 & 0 \\ 0 & -0.1 & 2.1 & -1 & -1 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & -1 & 2 \end{bmatrix}$$

Proposition

1. $L\mathbf{1} = \mathbf{0}$.
2. $\mathbf{x}^\top L\mathbf{x} = \sum_{\{i,j\}\in E} w_{i,j}(x_i - x_j)^2$, *which means* L *is PSD.*
3. $L\mathbf{x} = \mathbf{0} \iff \mathbf{x}^\top L\mathbf{x} = 0$.

Example

For $G = K_2 \dot\cup K_3 + \{2,3\}$,

$$\mathbf{x}^\top L\mathbf{x} = (x_1 - x_2)^2 + (x_3 - x_4)^2 + (x_4 - x_5)^2 + (x_3 - x_5)^2 + 0.1(x_2 - x_3)^2.$$

Count the number of components by the Laplacian matrix

Theorem (Fiedler 1973, Anderson and Morley 1971)

Let G be a graph and $L = L(G)$. Then $\operatorname{null}(L)$ is the number of components of G, and

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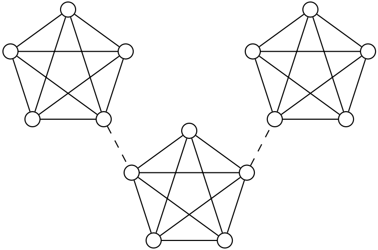
where $X_1, \ldots, X_k$ are the vertex sets of the components of G.

Example

For $G = K_2 \dot\cup K_3 + \{2, 3\}$,

$$\operatorname{spec}(L) = \{0, 0.08, 2.05, 3, 3.07\} \text{ and } \ker(L) = \operatorname{span}\left\{\begin{bmatrix}1\\1\\1\\1\\1\end{bmatrix}\right\}.$$



$\text{spec}(L) = \{0, 0.02, 0.06, 5, \ldots\}$ and $\ker(L) = \{\mathbf{1}\}$.

Just a small perturbation: first few eigvals and eigvecs

$$\{0,0,0\} \to \{0,0.02,0.06\}$$

$$\begin{bmatrix} 0.45 & 0 & 0 \\ 0.45 & 0 & 0 \\ 0.45 & 0 & 0 \\ 0.45 & 0 & 0 \\ 0.45 & 0 & 0 \\ 0 & 0.45 & 0 \\ 0 & 0.45 & 0 \\ 0 & 0.45 & 0 \\ 0 & 0.45 & 0 \\ 0 & 0.45 & 0 \\ 0 & 0 & 0.45 \\ 0 & 0 & 0.45 \\ 0 & 0 & 0.45 \\ 0 & 0 & 0.45 \\ 0 & 0 & 0.45 \end{bmatrix} \to \begin{bmatrix} 0.26 & 0.32 & -0.18 \\ 0.26 & 0.32 & -0.18 \\ 0.26 & 0.32 & -0.18 \\ 0.26 & 0.32 & -0.18 \\ 0.26 & 0.31 & -0.17 \\ 0.26 & 0.01 & 0.36 \\ 0.26 & -0.00 & 0.37 \\ 0.26 & -0.00 & 0.37 \\ 0.26 & -0.00 & 0.37 \\ 0.26 & -0.01 & 0.36 \\ 0.26 & -0.31 & -0.17 \\ 0.26 & -0.32 & -0.18 \\ 0.26 & -0.32 & -0.18 \\ 0.26 & -0.32 & -0.18 \\ 0.26 & -0.32 & -0.18 \end{bmatrix}$$

Count the number of clusters by the Laplacian matrix

Theorem

Let G be a weighted graph and $L = L(G)$. Then the number of zeroish eigenvalues suggests the number of clusters of G, and vertices in the same cluster share similar values in each eigenvector.

Example

For $G = K_2 \dot\cup K_3 + \{2,3\}$,

$$\operatorname{spec}(L) = \{0, 0.08, 2.05, 3, 3.07\} \text{ and } 0, 0.08 \to \begin{bmatrix} 0.45 \\ 0.45 \\ 0.45 \\ 0.45 \\ 0.45 \end{bmatrix}, \begin{bmatrix} 0.57 \\ 0.52 \\ 0.35 \\ 0.37 \\ 0.37 \end{bmatrix}$$

Spectral embedding algorithm

Algorithm

Input: a *weighted graph G* on n vertices and a *targeted dimension d*

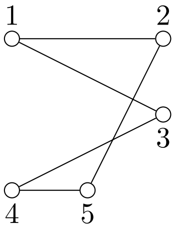
Output: an *$n \times d$ matrix Y*

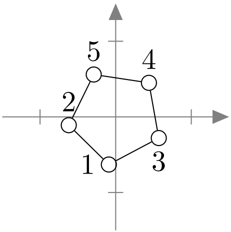
Steps:

1. $L \leftarrow L(G)$.
2. *Find the first d eigenvalues $\lambda_1 \leq \cdots \leq \lambda_d$ and the corresponding eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_d$.*
3. $Y \leftarrow$ *the matrix composed of columns $\mathbf{u}_1, \ldots, \mathbf{u}_d$.*
4. *Let $\mathbf{y}_1, \ldots, \mathbf{y}_n$ be the rows of Y. Define the embedding $f : V(G) \rightarrow \mathbb{R}^d$ by $i \mapsto \mathbf{y}_i$.*

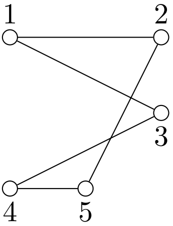
Remark

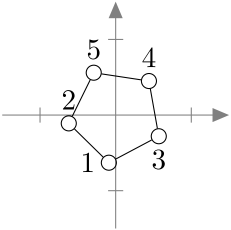
1. Since $\mathbf{u}_1 = \frac{1}{\sqrt{n}}\mathbf{1}$, people often take $\lambda_2 < \cdots < \lambda_{d+1}$ and their eigenvectors instead.
2. Main idea: *The embedding try to put adjacent vertices together—the stronger the weight, the closer they are.*





$$L = \begin{bmatrix} 2 & -1 & -1 & 0 & 0 \\ -1 & 2 & 0 & 0 & -1 \\ -1 & 0 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & -1 & 0 & -1 & 2 \end{bmatrix} \to Y = \begin{bmatrix} -0.09 & -0.63 \\ -0.62 & -0.11 \\ 0.57 & -0.28 \\ 0.44 & 0.45 \\ -0.29 & 0.56 \end{bmatrix}$$





The spectral embedding algorithm occurs in

- graph drawing (Hall 1970, Koren 2005),
- graph partitioning (Pothen, Simon, and Liou 1990),
- graph ordering (Juvan and Mohar 1992),
- spectral clustering (Shi and Malik 2000),
- Laplacian eigenmap (Belkin and Niyogi 2003),
- and more.

How to draw a graph properly?

Problem

Given a weighted graph G on n vertices and a target dimension d, find an $n \times d$ matrix Y such that

$$\begin{aligned} \textbf{minimize} \quad & \operatorname{tr}(Y^\top L Y) = \textstyle\sum_{\{i,j\} \in E(G)} \|\mathbf{y}_i - \mathbf{y}_j\|^2 \\ \textbf{subject to} \quad & \mathbf{1}^\top Y = \mathbf{0}^\top \textit{ and} \\ & Y^\top Y = I. \end{aligned}$$

Intuition:

- $\operatorname{tr}(T^\top L Y)$: the potential energy of a spring-mass system.
- $\mathbf{1}^\top Y = \mathbf{0}^\top$: centered at the origin.
- $Y^\top Y = I$: normalized each coordinate.

Spectral embedding algorithm generates the answer!

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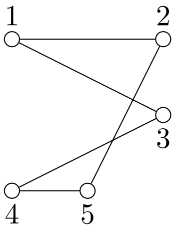
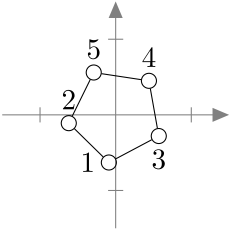
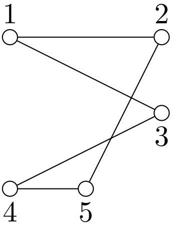
Some exmples

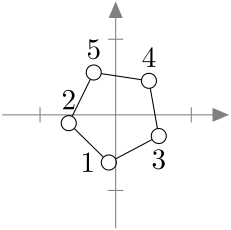




$$L = \begin{bmatrix} 2 & -1 & -1 & 0 & 0 \\ -1 & 2 & 0 & 0 & -1 \\ -1 & 0 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & -1 & 0 & -1 & 2 \end{bmatrix} \to Y = \begin{bmatrix} -0.09 & -0.63 \\ -0.62 & -0.11 \\ 0.57 & -0.28 \\ 0.44 & 0.45 \\ -0.29 & 0.56 \end{bmatrix}$$

Thanks!





$$L = \begin{bmatrix} 2 & -1 & -1 & 0 & 0 \\ -1 & 2 & 0 & 0 & -1 \\ -1 & 0 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & -1 & 0 & -1 & 2 \end{bmatrix} \to Y = \begin{bmatrix} -0.09 & -0.63 \\ -0.62 & -0.11 \\ 0.57 & -0.28 \\ 0.44 & 0.45 \\ -0.29 & 0.56 \end{bmatrix}$$

Thanks!

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