Introduction to spectral graph theory

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Aalto 2021

Outline

Motivation

Review of spectral graph theory

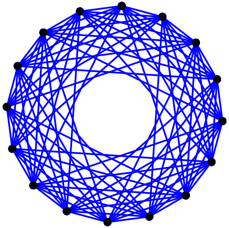
Motivation

Spectral graph theory

Spectral graph theory is concerned with the study of matrices related to graphs.

Applications:

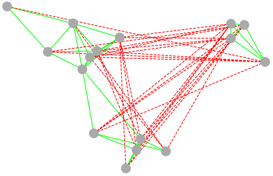
- Visualization.
- Combinatorial optimization.
  - Coloring.
  - Finding dense subgraphs.
- Clustering.
- Analysis of random walks.



Spectral graph theory

Signed graphs:

- Fundamental differences with respect to unsigned graphs. E.g.:
  - It can be hard to find shortest paths.
  - It can be hard to find densest subgraphs.
  - Graph Laplacians can be non-singular.
- Currently a hot-topic. Some applications:
  - Conflict in social networks.
  - User-item ratings.
  - Protein interactions.
  - Geopolitics.



Spectral graph theory

Consider a symmetric matrix $A \in \mathbb{R}^{n \times n}$.

An eigenvector $v \in \mathbb{R}^n$ of A satisfies $Av = \lambda v$ for some $\lambda \in \mathbb{R}$.

λ is an eigenvalue of A.

Spectral graph theory

Consider a symmetric matrix $A \in \mathbb{R}^{n \times n}$.

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λ is an eigenvalue of A.

Eigenvalue decomposition: for every real symmetric matrix A we can write

$$A = V \Lambda V^{-1},$$

where

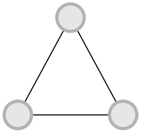
- V is orthogonal (i.e. $VV^T = V^T V = I$),
- the columns of V are eigenvectors of A,
- Λ is diagonal and the elements in its main diagonal are eigenvalues of A.

Review of spectral graph theory

We consider simple undirected graphs with no loops.

$G = (V, E), E \subseteq \{(i, j) : i, j \in V\}, (i, j) = (j, i).$

Adjacency matrix: $A_{ij} = \begin{cases} 1 & \text{if } (i, j) \in E \\ 0 & \text{otherwise} \end{cases}$

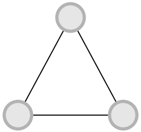


$$\mapsto \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

Spectral graph theory

Graph Laplacian: $L = D - A$.

Degree matrix: $D_{ij} = \begin{cases} d_i & \text{if } i = j \;\; (d_i \text{ is the degree of vertex } i) \\ 0 & \text{otherwise} \end{cases}$



$$\mapsto \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}$$

Spectral graph theory

Can you think of an eigenvector of L?

$v = (\qquad)^T$.

$$\begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix} \begin{pmatrix} \\ \\ \\ \end{pmatrix} = \begin{pmatrix} \\ \\ \\ \end{pmatrix}$$

Reminder

$Av = \lambda v$ for some $\lambda \in \mathbb{R}$.

Spectral graph theory

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Spectral graph theory

Can you think of an eigenvector of L?
$v = (1, 1, 1)^T$.

Reminder

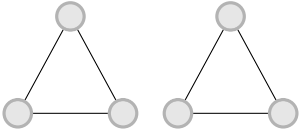
$Av = \lambda v$ for some $\lambda \in \mathbb{R}$.

$$\begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} = 0v$$

For any graph, $v = (1, 1, \ldots, 1)^T$ is always an eigenvector of L, with eigenvalue 0.

Spectral graph theory

Another graph (2 connected components):



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

Spectral graph theory

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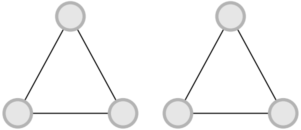

$$\begin{pmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & -1 & -1 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & -1 & 2 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0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

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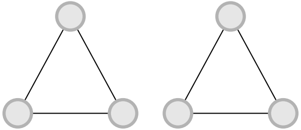


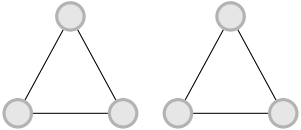
$$\begin{pmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & -1 & -1 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & -1 & 2 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0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

The multiplicity of eigenvalue 0 in L is equal to the number of connected components.

$v_1 = (1, 1, 1, 0, 0, 0)^T$ and $v_2 = (0, 0, 0, 1, 1, 1)^T$ are eigenvectors with eigenvalues $\lambda_1 = \lambda_2 = 0$.

Spectral graph theory

Another graph (2 connected components):



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

Reminder

If $v1$, $v2$ satisfy
$Lv_1 = \lambda v_1$,
$Lv_2 = \lambda v_2$, then
$u = \alpha v_1 + \beta v_2$
satisfies $Lu = \lambda u$.

The multiplicity of eigenvalue 0 in L is equal to the number of connected components.

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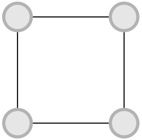
Spectral graph theory

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



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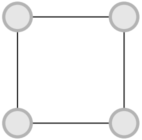

Spectrum: $(-2, 0, 0, 2)$

Spectral graph theory

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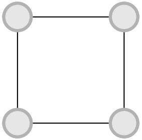
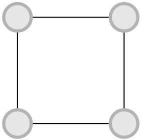


Spectrum: $(-2, 0, 0, 2)$

Eigenvectors: $\begin{pmatrix} -1 & 0 & 1 & -1 \\ 1 & 1 & -0 & -1 \\ -1 & -0 & -1 & -1 \\ 1 & -1 & 0 & -1 \end{pmatrix}$

Spectral graph theory

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



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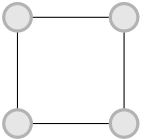

Spectrum: ?

Spectral graph theory

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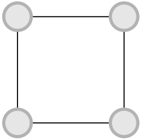

Spectrum: $(0, 2, 2, 4)$

Spectral graph theory

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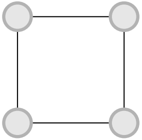

Spectrum: $(0, 2, 2, 4)$

Eigenvectors:?

Spectral graph theory

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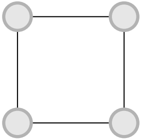

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Eigenvectors: $\begin{pmatrix} -1 & 0 & 1 & -1 \\ 1 & 1 & -0 & -1 \\ -1 & -0 & -1 & -1 \\ 1 & -1 & 0 & -1 \end{pmatrix}$

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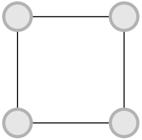

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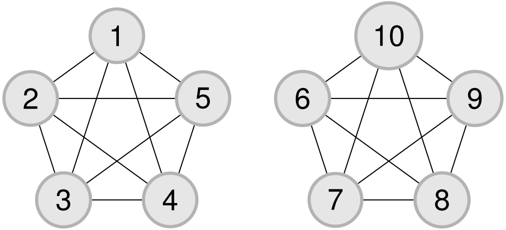
Eigenvectors: $\begin{pmatrix} -1 & 0 & 1 & -1 \\ 1 & 1 & -0 & -1 \\ -1 & -0 & -1 & -1 \\ 1 & -1 & 0 & -1 \end{pmatrix}$

Reminder

If $Av = \lambda v$, then $(\alpha A + \beta I)v = (\alpha\lambda + \beta)v$.

Spectral graph theory

Fiedler vector, v_2, corresponding to the second smallest eigenvalue, λ_2, of the Laplacian.



$v_2 =$

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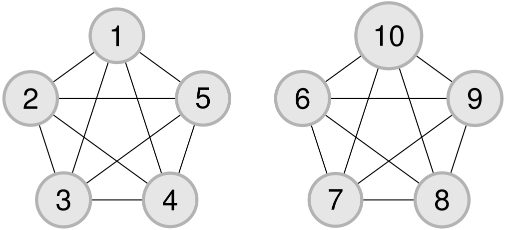
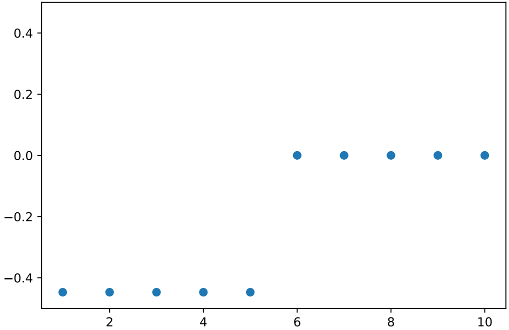




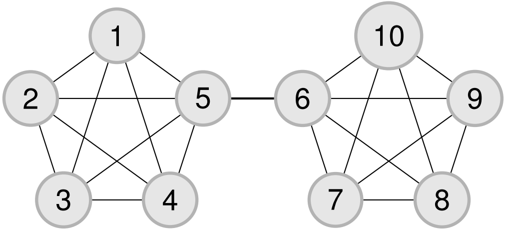
$v_2 =$

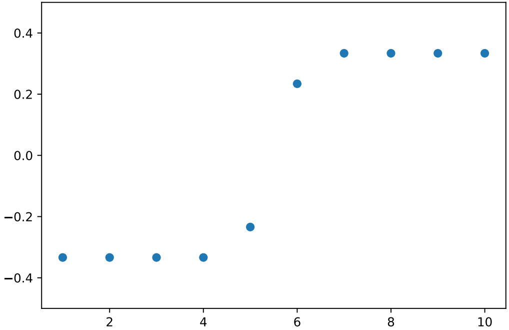
$$(-0.447, -0.447, -0.447, -0.447, -0.447, 0, 0, 0, 0, 0)$$

$\lambda_2 = 0$

Spectral graph theory

Fiedler vector, v_2, corresponding to the second smallest eigenvalue, λ_2, of the Laplacian.



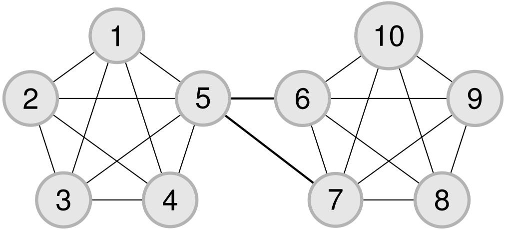


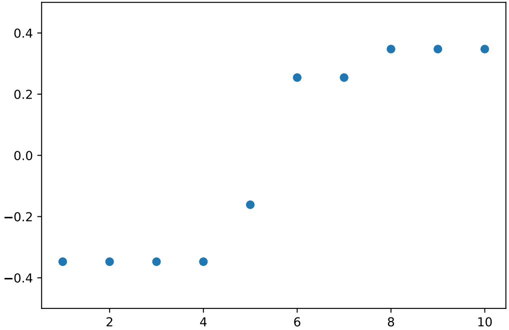
$v_2 =$
$(-0.334, \ -0.334, \ -0.334, \ -0.334, \ -0.234, \ 0.234, \ 0.334, \ 0.334, \ 0.334, \ 0.334)$

$\lambda_2 \approx 0.298$

Spectral graph theory

Fiedler vector, v_2, corresponding to the second smallest eigenvalue, λ_2, of the Laplacian.



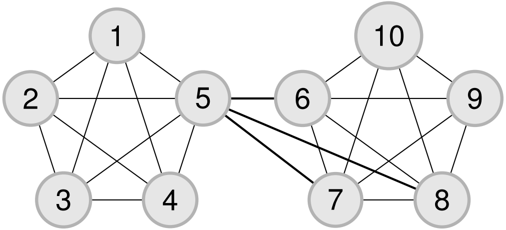


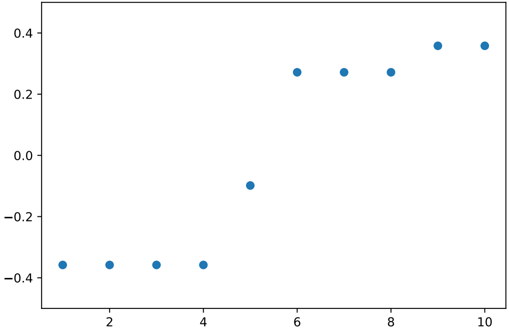
$v_2 =$
$(-0.347, -0.347, -0.347, -0.347, -0.161, 0.254, 0.254, 0.347, 0.347, 0.347)$

$\lambda_2 \approx 0.535$

Spectral graph theory

Fiedler vector, v_2, corresponding to the second smallest eigenvalue, λ_2, of the Laplacian.



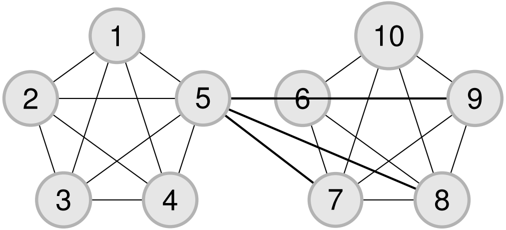


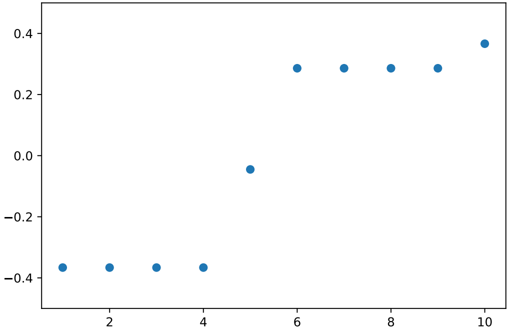
$v_2 =$
$(-0.358, \ -0.358, \ -0.358, \ -0.358, \ -0.098, \ 0.272, \ 0.272, \ 0.272, \ 0.358, \ 0.358)$

$\lambda_2 \approx 0.725$

Spectral graph theory

Fiedler vector, v_2, corresponding to the second smallest eigenvalue, λ_2, of the Laplacian.





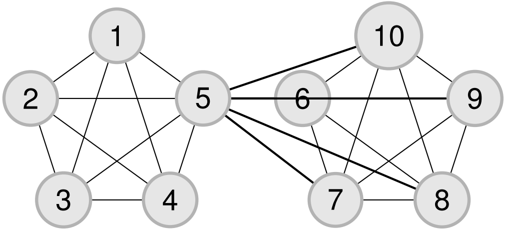
$v_2 =$

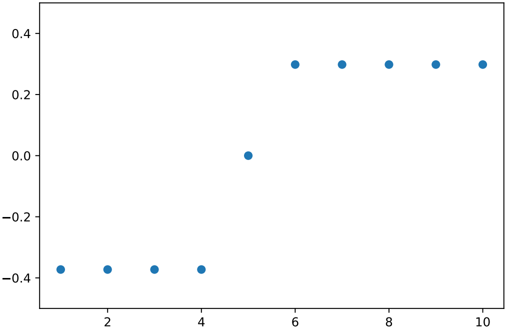
$(-0.366, -0.366, -0.366, -0.366, -0.045, 0.286, 0.286, 0.286, 0.286, 0.366)$

$\lambda_2 \approx 0.876$

Spectral graph theory

Fiedler vector, v_2, corresponding to the second smallest eigenvalue, λ_2, of the Laplacian.





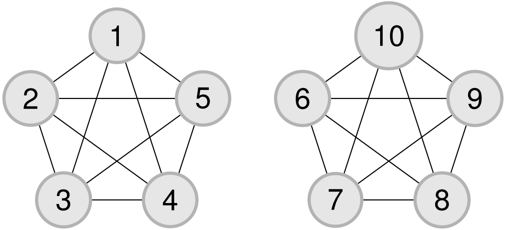
$v_2 =$

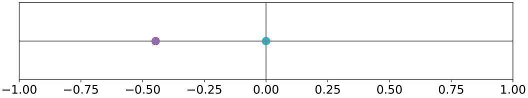
$(-0.373, \; -0.373, \; -0.373, \; -0.373, \; 0., \; 0.298, \; 0.298, \; 0.298, \; 0.298, \; 0.298)$

$\lambda_2 \approx 1$

Spectral graph theory

Application: clustering.





Points in $\mathbb{R}$.

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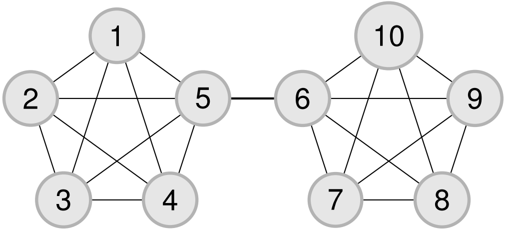
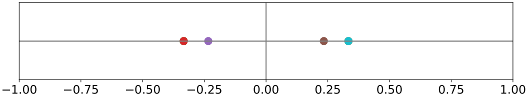
$(-0.447, -0.447, -0.447, -0.447, -0.447, 0, 0, 0, 0, 0)$

Spectral graph theory

Application: clustering.



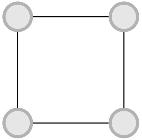


Points in $\mathbb{R}$.

$$v_2 = (-0.334,\ -0.334,\ -0.334,\ -0.334,\ -0.234,\ 0.234,\ 0.334,\ 0.334,\ 0.334,\ 0.334)$$

Spectral graph theory

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

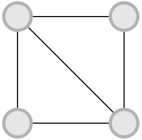


Some properties of the Laplacian matrix:

- L is positive semidefinite (P.S.D.), i.e. $x^T L x \geq 0$ for all $x \in \mathbb{R}^n$. Equivalently, $\lambda_i \geq 0$ for all i.
- The multiplicity of the eigenvalue 0 equals the number of connected components.

Spectral graph theory

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



Some properties of the adjacency matrix:

- λ_{max} ? d_{avg}.

Spectral graph theory

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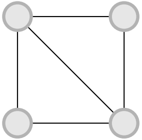

Some properties of the adjacency matrix:

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Spectral graph theory

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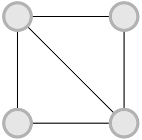

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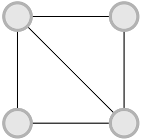

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Spectral graph theory

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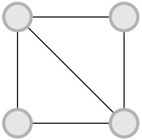

Some properties of the adjacency matrix:

- $\lambda_{max} \geq d_{avg}$.
- $\lambda_{max} \leq d_{max}$.
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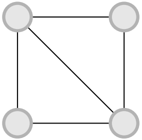

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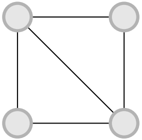

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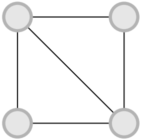

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Reminder

$Tr(A) = \sum_i \lambda_i$.

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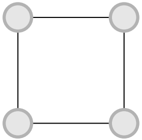

Spectrum: $(-2, 0, 0, 2)$

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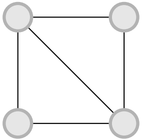

Spectrum: ?

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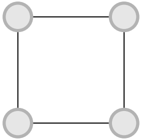

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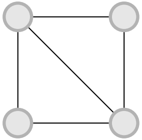

Spectrum: $(-1.562, -1, 0, 2.562)$

Spectral graph theory

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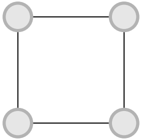

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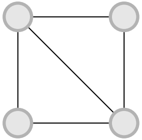

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Reminder

$\|A\|_F^2 = \sum_i \sum_j a_{ij}^2 = \sum_i \lambda_i^2.$

Spectral graph theory

Take-aways from this lecture:

- Adjacency matrix and some of its properties.
- Graph Laplacian and some of its properties.
- Fiedler vectors.
- Linear algebra concepts:
  - The eigenvalue decomposition of a matrix.
  - Eigenvectors and eigenvalues: $Av = \lambda v$ for some $\lambda \in \mathbb{R}$.
  - If $v1, v2$ satisfy $Lv_1 = \lambda v_1$, $Lv_2 = \lambda v_2$, then $u = \alpha v_1 + \beta v_2$ satisfies $Lu = \lambda u$.
  - If $Av = \lambda v$, then $(\alpha A + \beta I)v = (\alpha\lambda + \beta)v$.
  - $Tr(A) = \sum_i \lambda_i$.
  - $\|A\|_F^2 = \sum_i \sum_j a_{ij}^2 = \sum_i \lambda_i^2$.