Objectives

Spectral Graph Theory

- The Quadratic Form
- Laplacian characterization

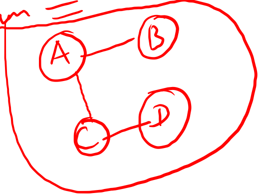
Quadratic Form of Laplacian

The Laplacian of an edge

Definition: Let L_e be the Laplacian of the graph on n vertices consisting of just the edge e. If e is the edge (v_1, v_2), then

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

row sum $\Longrightarrow 0$



By additivity, we can write the Laplacian of graph with many edges:

$$L_G = \sum_{e \in E} L_e$$

$L \cdot x = 0 \cdot x$

- The above concept could be used to prove many facts; proving them for one edge and adding them up.

QUADRATIC FORM OF LAPLACIAN ..

From

$$L_G = \sum_{e \in E} L_e$$

- So, for an edge e, $L_e = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \oplus [zeros]$
- Let's decompose L_e as $\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \begin{pmatrix} 1 & -1 \end{pmatrix}$
- Normalizing vectors will yield $L_e = 2 \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix}$, so, $(\frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}})^T$ is an eigenvector with eigenvalue 2.
- We will extend above to compute $x^T L_e x = \begin{pmatrix} x_1 & x_2 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \begin{pmatrix} 1 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = (x_1 - x_2)^2$

THE QUADRATIC FORM

- The Laplacian is a quadratic form, specifically:

$$x^T L_G x = x^T \Big(\sum_{e \in E} L_e\Big) x = \sum_{e \in E} x^T L_e x = \boxed{\sum_{(i,j) \in E} (x_i - x_j)^2}$$

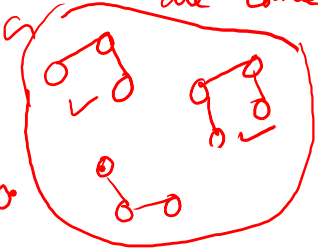
Use Laplacian for partitioning $\underline{\underline{G}}$

Smallest eigen value $\lambda_1 = 0$ or same value
$\lambda_2 = 0$ $\Big\} \Rightarrow$ indicates G is disconnected
G have 2 components that are connected.

$\lambda_3 = 0$

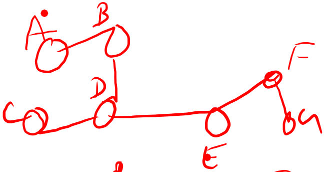
algebraic multiplicity of $\underline{\underline{0}}$ is $\underline{\underline{3}}$

So there are 3 connected components



$\lambda_1 = 0$

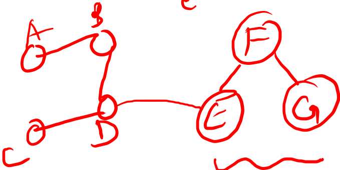
$\lambda_1 \le \lambda_2 \le \lambda_3$
$\underline{\lambda_1} = 0$



λ_2

minimum edges bet^n the subgraph

→ Cut minimal



Connect^n within subgraph is high

Finding λ_2 as optimization problem.

$L \cdot x = \underline{\underline{\lambda}} \cdot x$

$$\lambda_2 = \min_x \frac{x^T L x}{x^T x} \rightarrow$$

for any symmetric matrix L

$A_{23} = 1$ if $A_{ij} = 1$

$A_{32} = 1$ $\quad A_{ji} = 1$

Meaning of $\min_x x^T L x$ on G

labels or values for nodes

$$x^T L x = \sum_{i,j=1}^n L_{ij} x_i x_j = \sum_{i,j=1}^n (D_{ij} - A_{ij}) x_i \cdot x_j$$

$$= \sum_{i,j=1}^n D_{ij} x_i \cdot x_j - \sum_{i,j=1}^n A_{ij} x_i x_j$$

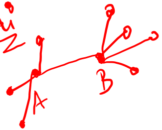
$$= \sum_{i,j=1}^n D_{ii} x_i x_i - \sum_{i,j \in E} 2 x_i \cdot x_j$$

x_i^2

$$= \sum_{(i,j) \in E} (x_i^2 + x_j^2 - 2 x_i \cdot x_j)$$

$$= \sum (x_i - x_j)^2$$

Node i has degree d_i



D [ ]

$$\lambda_2 = \min_{x} \frac{x^T L x}{x^T x}.$$

$$\lambda_2 = \min_{x} \frac{\sum_{(i,j) \in E} (x_i - x_j)^2}{\sum_i x_i^2 = 1}$$

s.t. $\sum x_i = 0$

x_i

Assign values x_i to node i such that few edges cross $\underline{0}$ value

SYMMETRIC AND POSITIVE SEMIDEFINITE

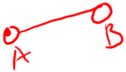
n vertices

- Prove that L is symmetric and positive semidefinite
  - $L = D - A$; L is symmetric since it follows symmetry of D and A
  - From the quadratic form $x^T L x = \sum_{(i,j) \in E} (x_i - x_j)^2$, hence $x^T L x \geq 0, \forall x \in \mathbb{R}^n$.

    > 0

    This implies that L is positive semidefinite.

    Note: All eigenvalues will be ≥ 0



labels/values assigned to nodes.

EIGENVALUE 0

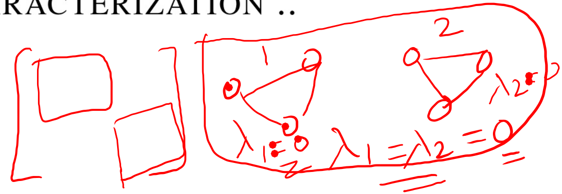
- Show that for every graph G, there is an eigenvector of L_G with eigenvalue 0.

  Proof: Consider the quadratic form $x^T L x = \sum_{(i,j)\in E} (x_i - x_j)^2$, the only way this quadratic form can be zero is if $x_i = x_j$ whenever there is an edge (i,j). In other words, this quadratic form is zero iff $x_i = x_j$ for every i and j in the same connected component.

  The corresponding eigenvector is a constant vector; for example, $\mathbf{1}$ is eigenvector of 1's, then $L\mathbf{1} = 0\mathbf{1}$, which implies eigenvalue is 0.

$L \cdot 1 = 0 \cdot 1$

row sum / col. sum = 0



MULTIPLICITY IN EIGEN VALUES

- A graph G has k connected components iff the algebraic multiplicity of 0 in the Laplacian is k.

  Proof: G has k connected components iff Laplacian matrix has k blocks. Let the blocks be denoted $L_1, \ldots, L_k$.

  Each block matrix in the Laplacian has eigenvalue 0.

  $L_{(1 \cup 2 \cup \ldots k)}$ has combined eigen values of $L_1, \ldots, L_k$.

  Therefore, the eigenvalues of L contain 0 with a multiplicity of k.

$L = \sum_e L_e$

OBJECTIVES

SPECTRAL GRAPH THEORY

- Graph Partitioning

$$\lambda_2 = \min_{x} \frac{x^T L x}{x^T x} \rightarrow \sum_{(i,j) \in E} (x_i - x_j)^2$$

$$\lambda_2 = \min \frac{\sum_{(i,j)\in E} (x_i - x_j)^2}{\sum x_i^2 = 1}$$

All the labellings of nodes

$\sum x_i = 0$

$x \perp 1$

n vertices then n comps in x

$x \rightarrow$ eigenvector

$x \rightarrow$ unit vector

$\sum x_i^2 = 1$

$$\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

Eigenvectors are orthogonal to each other.

$x_1 \perp x_2 \perp x_3 \cdots$

Normal vector

$\sum x_i^2 = 1$

x_i : red or green

$x_i = +1$ or -1

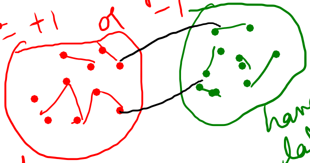
Min Cut

λ_2 : min x

$Lx = 0 \cdot x$

+1

-1



have label $x_i = +1$

have label $x_i = -1$

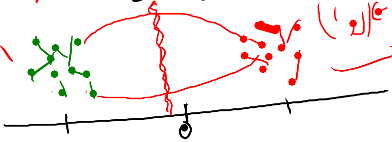
Edges that span across 0 should be as small as possible (Min cut)

$\sum x_i = 0$

$$\sum_{(i,j)\in E} (x_i - x_j)$$

$x_i = -1$

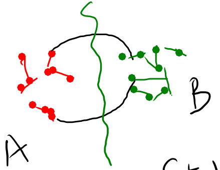
$\rightarrow x_i = +1$



0

x_i

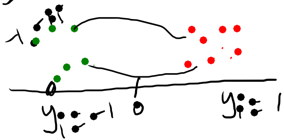
x_i's are equal/similar for same group



$$y_i = \begin{cases} +1, & i \in A \\ -1, & i \in B \end{cases}$$

We can minimize the cut of the partition by finding a vector x that minimizes

$$\underset{y_i \in [-1,+1]}{\arg\min} f(y) = \sum_{(i,j)\in E} (y_i - y_j)^2$$



Rayleigh Theorem

$$\min_{y \in \mathbb{R}^n} f(y) = \sum_{(i,j)\in E} (y_i - y_j)^2$$

$$= y^T L y$$

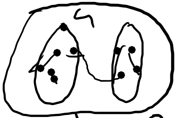
y_i $\underbrace{[-1, +1]}$.

$$\lambda_2 = \min_y f(y)$$

$$x = \arg\min_y f(y)$$

Spectral Clustering Algorithm

Input : Graph

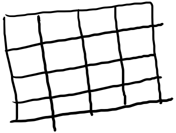


$\lambda_1 = 0$

$\lambda_2 = 0.02$

1) Preprocessing

Construct Laplacian matrix from G.



L

$$\lambda \quad \begin{bmatrix} 0.0 \\ 0.1 \\ 0.6 \\ 0.7 \end{bmatrix} \begin{matrix} \to \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \lambda_4 \end{matrix}$$

e_1	e_2	e_3	e_4
0.0	0.1	0.6	0.7

X.

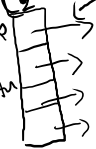
corr. eigen vector

2) Decomposition

Compute eigen vector and eigen values of matrix

Map each node(point) to a lower dim representation based on one or more eigen vector

X e_2



Map vertices to corr. eigen vector e_2

corr. to node 1

" 2

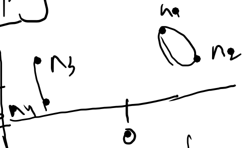
" 3

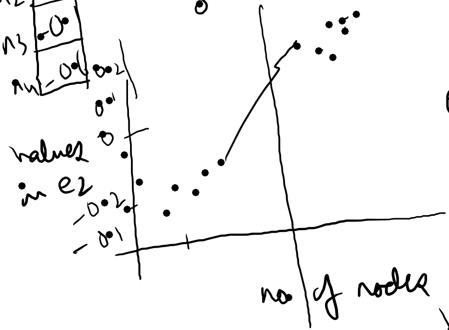
" 4

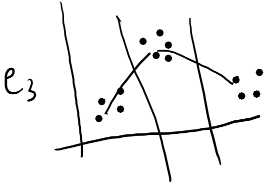
3. Grouping

	e_2
n_1	0.1
n_2	0.6
n_3	-0.
n_4	-0.6

2-partition





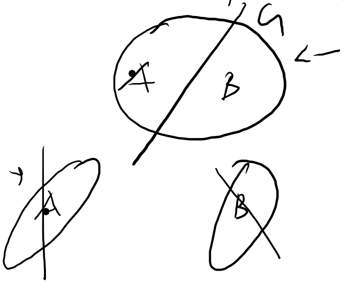


$\lambda_1 = 0 \quad \lambda_2 = 0.01 \quad \lambda_3 \; 0.2 \quad \lambda_4 \; 0.5$

K-way Spectral clustering

If K partitions/Clusters from G.

Recursive bi_partitioning



Bounding λ_2 and λ_{max} (1/2)

Courant-Fischer Formula

- The Courant-Fischer theorem gives a variational formulation of the eigenvalues of a symmetric matrix, which can be useful for obtaining bounds on the eigevalues.

$$\lambda_1 = \min_{||x||=1} x^T L x = \min_{x \neq 0} \frac{x^T L x}{x^T x}$$

$$\lambda_2 = \min_{||x||=1, x \perp v_1} x^T L x = \min_{x \perp v_1, x \neq 0} \frac{x^T L x}{x^T x}$$

$$\lambda_{max} = \max_{||x||=1} x^T L x = \max_{x \neq 0} \frac{x^T L x}{x^T x}$$

Bounding λ_2 and λ_{max} (2/2)

Rayleigh quotient

- The Rayleigh quotient is the application of the Courant-Fischer Formula to the Laplacian of a graph.

$$v_1 = \mathbf{1}, \lambda_1 = 0$$

$$\lambda_2 = \min_{x \perp v_1, x \neq 0} \frac{x^T L x}{x^T x} = \min_{x \perp v_1, x \neq 0} \frac{\sum\limits_{(i,j) \in E} (x_i - x_j)^2}{\sum\limits_{i \in V} x_i^2}$$

$$\lambda_{max} = \max_{x \neq 0} \frac{x^T L x}{x^T x} = \max_{x \neq 0} \frac{\sum\limits_{(i,j) \in E} (x_i - x_j)^2}{\sum\limits_{i \in V} x_i^2}$$

Graph Partitioning

Using λ_2

- We know that $\lambda_1 = 0,\ \upsilon_1 = \mathbf{1}$
- Since eigenvectors forms orthonormal basis, second eigenvector say x is orthogonal to the first one,
  - $x.\mathbf{1} = 0$, i.e $\sum_i x_i = 0$ and normal $\sum_i x_i^2 = 1$
- Also from Raleigh quotient,

$$\lambda_2 = \min_{x \perp \upsilon_1, x \neq 0} \frac{x^T L x}{x^T x} = \min_{x \perp \upsilon_1, x \neq 0} \frac{\sum_{(i,j) \in E} (x_i - x_j)^2}{\sum_{i \in V} x_i^2}$$

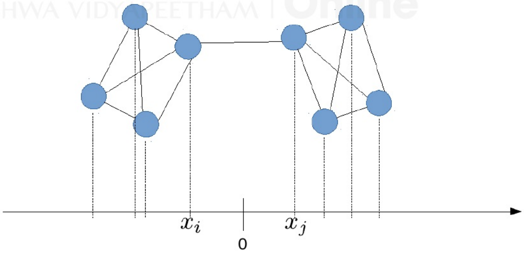
$$\lambda_2 = \min_{x : \sum_i x_i = 0} \sum_{(i,j) \in E} (x_i - x_j)^2$$

Graph Partitioning ..

$$\lambda_2 = \min_{x:\sum_i x_i = 0} \sum_{(i,j)\in E} (x_i - x_j)^2$$

What does it indicate

- Nodes should be placed at both sides of 0 because $\sum_i x_i = 0$



Objectives

Spectral Graph Theory

- Graph Partitioning Examples

The algebraic connectivity

because if k connected comp. are there $\lambda_1 = \lambda_2 = \cdots \lambda_k = 0$ $\lambda_{k+1} > 0$

Fiedler Number

- The first non-null eigenvalue λ_{k+1} is called the Fiedler value. λ_2
- The corresponding eigenvector v_{k+1} is called the Fiedler vector.
- The multiplicity of the Fiedler eigenvalue is always equal to 1.
- The Fiedler value is the algebraic connectivity of a graph, the further from 0, the more connected

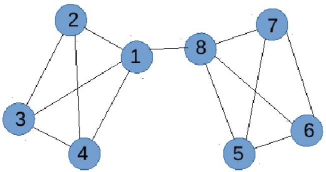
algebraic

Algebraic Multiplicity of a value b $= m$.

ie $\underset{=3}{m}$ eigenvalues have value b

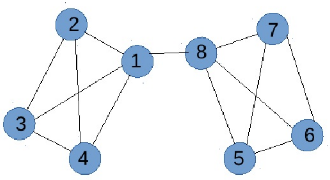
$\lambda_1 = b \quad \lambda_5 = b \quad \lambda_9 = b$

Graph Partitioning: Example 1



$$L = \begin{pmatrix} 4 & -1 & -1 & -1 & 0 & 0 & 0 & -1 \\ -1 & 3 & -1 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 3 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & -1 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & -1 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 3 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & -1 & 3 & -1 \\ -1 & 0 & 0 & 0 & -1 & -1 & -1 & 4 \end{pmatrix}$$

GRAPH PARTITIONING: EXAMPLE 1 ..



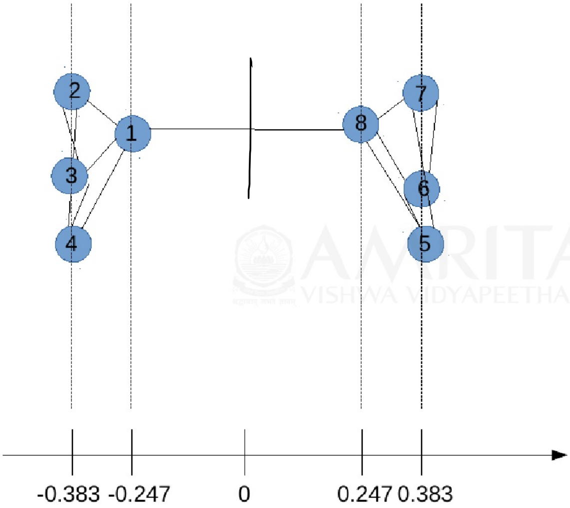
Fiedler value

$\lambda_1 = 0, \; \lambda_2 = 0.354$

Fiedler vector

$$L = \begin{pmatrix} 4 & -1 & -1 & -1 & 0 & 0 & 0 & -1 \\ -1 & 3 & -1 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 3 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & -1 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & -1 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 3 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & -1 & 3 & -1 \\ -1 & 0 & 0 & 0 & -1 & -1 & -1 & 4 \end{pmatrix} \qquad v_2 = \begin{pmatrix} 0.247 \\ 0.383 \\ 0.383 \\ 0.383 \\ -0.383 \\ -0.383 \\ -0.383 \\ -0.247 \end{pmatrix}$$

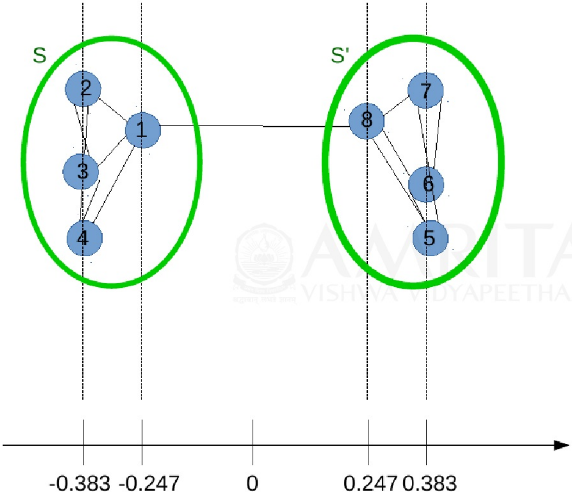
Graph Partitioning: Example 1 ..



$\lambda_1 = 0,\ \lambda_2 = 0.354$

$$v_2 = \begin{pmatrix} 0.247 \\ 0.383 \\ 0.383 \\ 0.383 \\ -0.383 \\ -0.383 \\ -0.383 \\ -0.247 \end{pmatrix} \begin{array}{l} n_5 \\ n_6 \\ n_7 \\ n_8 \\ n_4 \\ n_2 \\ n_3 \\ n_1 \end{array}$$

Graph Partitioning: Example 1 ...

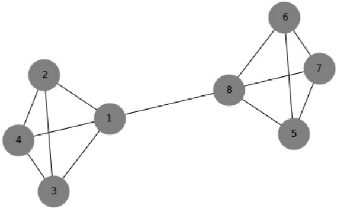


$\lambda_1 = 0, \ \lambda_2 = 0.354$

$$\upsilon_2 = \begin{pmatrix} 0.247 \\ 0.383 \\ 0.383 \\ 0.383 \\ -0.383 \\ -0.383 \\ -0.383 \\ -0.247 \end{pmatrix}$$

EXAMPLE 1: JUPYTER

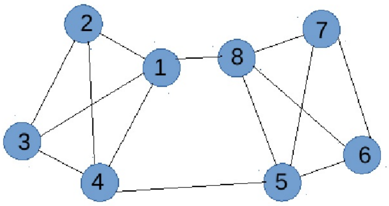
```python
import networkx as nx
import numpy as np
import matplotlib.pyplot as plt
from numpy import linalg as LA
np.set_printoptions(precision=3)
GP1=nx.Graph([(1,2),(1,3),(1,4),(2,3),(2,3),(2,4
(5,6),(5,7),(5,8),(6,7),(6,8),(7,8), (1,8)])
nx.draw(GP1, node_size = 1500, node_color="", w
plt.show()
S= nx.laplacian_matrix(GP1)
T=S.todense()
print(T)
evals, evecs = LA.eig(T)
evals=evals.real
print(evals)
evecs=evecs.real
print(evecs)
```




```
[  5.64     0     0.354   4.0     4.0     4.0     4.0     4.0]

[[ 0.663  −0.354  −0.247  −0.612   0.344   0.04    0.072  −0.314]
 [−0.143  −0.354  −0.383   0.204   0.416  −0.251   0.105  −0.479]
 [−0.143  −0.354  −0.383   0.204  −0.563  −0.223   0.526   0.314]
 [−0.143  −0.354  −0.383   0.204  −0.197   0.434  −0.703   0.48 ]
 [ 0.143  −0.354   0.383   0.204  −0.295   0.567  −0.105  −0.064]
 [ 0.143  −0.354   0.383   0.204  −0.295  −0.613  −0.296  −0.101]
 [ 0.143  −0.354   0.383   0.204   0.246   0.006   0.33    0.479]
 [−0.663  −0.354   0.247  −0.612   0.344   0.04    0.072  −0.314]]
```

Graph Partitioning: Example 2 ..



$\lambda_1 = 0,\ \lambda_2 = 0.764$

$$L = \begin{pmatrix} 4 & -1 & -1 & -1 & 0 & 0 & 0 & -1 \\ -1 & 3 & -1 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 3 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & -1 & 4 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 4 & -1 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 3 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & -1 & 3 & -1 \\ -1 & 0 & 0 & 0 & -1 & -1 & -1 & 4 \end{pmatrix} \qquad v_2 = \begin{pmatrix} 0.263 \\ 0.425 \\ 0.425 \\ 0.263 \\ -0.263 \\ -0.425 \\ -0.425 \\ -0.263 \end{pmatrix}$$

SUMMARY

SPECTRAL GRAPH THEORY

- Graph Partitioning Examples
- Fiedler Number

References

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Linear algebra, 2013.

Strang, G.
Linear algebra and its applications.
Belmont, CA: Thomson, Brooks/Cole, 2006.