

Spectral graph clustering

Mining Massive Datasets

Carlos Castillo

Topic 12



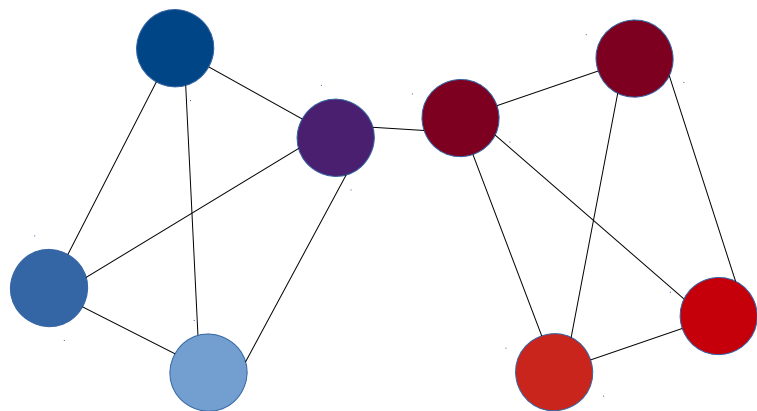
Universitat
Pompeu Fabra
Barcelona

Sources

- **Jure Leskovec (2016)**
Defining the graph laplacian [video]
- Evimaria Terzi: **Graph cuts** / spectral graph partitioning
- Daniel A. Spielman (2009): **The Laplacian**
- C. Castillo (2017) **Graph partitioning**

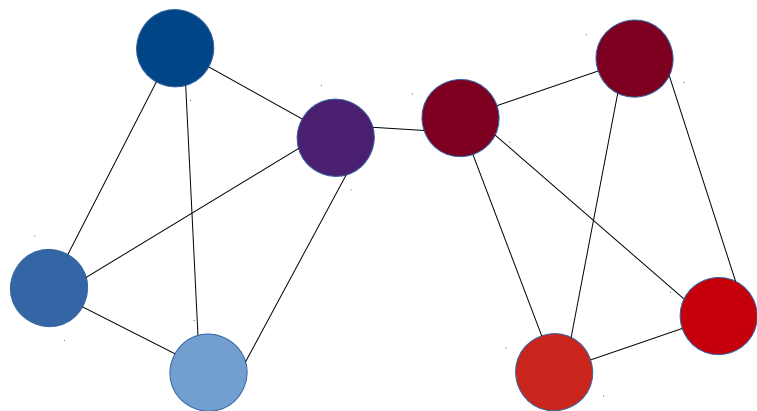
Graphs are nice, but ...

- They describe only local relationships
- We would like to understand a global structure
- Our objective is transforming a graph into a more familiar object: a cloud of points in \mathbb{R}^k



Graphs are nice, but ...

- They describe only local relationships
- We would like to understand a global structure
- Our objective is transforming a graph into a more familiar object: a cloud of points in \mathbb{R}^k



Distances should be somehow preserved

What is a graph embedding?

- A graph embedding is a mapping from a graph to a vector space
- If the vector space is \mathbb{R}^2 you can think of an embedding as a way of drawing a graph

Try drawing this graph

$$V = \{v1, v2, \dots, v8\}$$

$$E = \{ (v1, v2), (v2, v3), (v3, v4), (v4, v1), (v5, v6), (v6, v7), (v7, v8), (v8, v5), (v1, v5), (v2, v6), (v3, v7), (v4, v8) \}$$

Draw this graph on paper

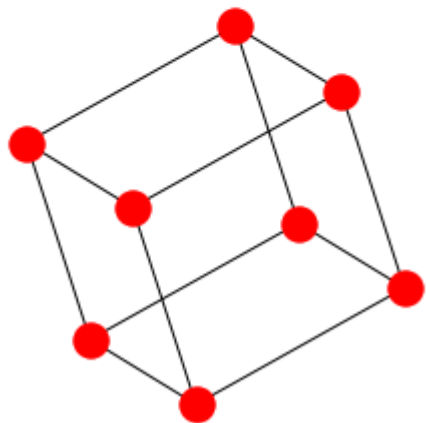
What constitutes a good drawing?

2D graph embeddings in NetworkX

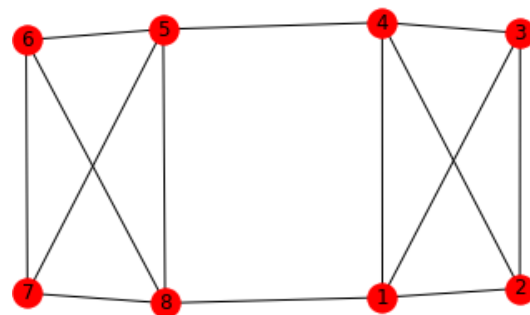


```
import matplotlib.pyplot as plt
import networkx as nx

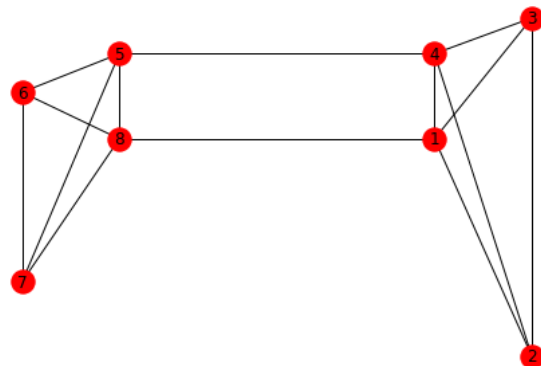
plt.figure(figsize=(3,3))
G = nx.hypercube_graph(3)
nx.draw_spectral(G)
_ = plt.show()
```



`nx.draw_networkx(g)`



`nx.draw_spectral(g)`



In a good graph embedding ...

- Pairs of nodes that are **connected** to each other should be **close**
- Pairs of nodes that are **not connected** should be **far**
- **Compromises usually need to be made**

Random 2D graph projection

- Start a BFS from a random node, that has $x=1$, and nodes visited have ascending x
- Start a BFS from another random node, which has $y=1$, and nodes visited have ascending y
- Project node i to position (x_i, y_i)

How do you think this works in practice?

Eigenvectors of adjacency matrix

Adjacency matrix of $G=(V,E)$

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

- What is Ax ? Think of x as a set of labels/values:

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ a_{21} & \dots & a_{2n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

$$y_i = \sum_{j:(j,i) \in E} x_j$$

Ax is a vector whose i^{th} coordinate contains the sum of the x_j who are in-neighbors of i

Properties of adjacency matrix

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

- How many non-zeros are in every row of A ?

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ a_{21} & \dots & a_{2n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \dots & a_{nn} \end{bmatrix}$$

Understanding the adjacency matrix

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

What is Ax ? Think of x as a set of labels/values:

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ a_{21} & \dots & a_{2n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

Ax is a vector whose i^{th} coordinate contains the sum of the x_j who are in-neighbors of i

$$y_i = \sum_{j:(j,i) \in E} x_j$$

Spectral graph theory

- The study of the eigenvalues and eigenvectors of a graph matrix
 - Adjacency matrix $Ax = \lambda x$
 - Laplacian matrix (next)
- Suppose graph is d -regular, $k_i = d \ \forall i$ what is the value of:
- What does that imply?

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ a_{21} & \dots & a_{2n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} = ?$$

An easy eigenvector of A

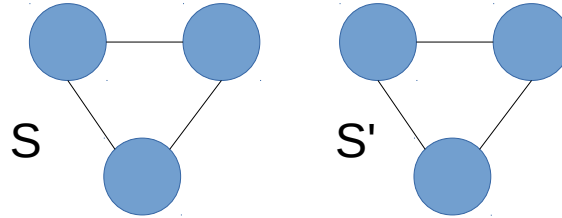
- Suppose graph is d -regular, i.e. all nodes have degree d :

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ a_{21} & \dots & a_{2n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} = \begin{bmatrix} d \\ d \\ \vdots \\ d \end{bmatrix} = d \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}$$

- So $[1, 1, \dots, 1]^\top$ is an eigenvector of eigenvalue d

Disconnected graphs

- Suppose graph is disconnected (still regular)

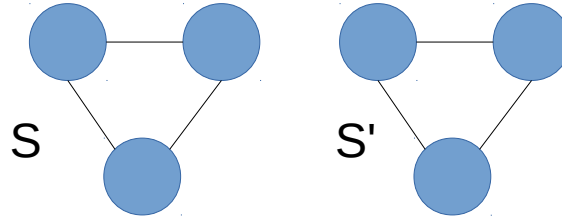


- Then its adjacency matrix has block structure:

$$A = \begin{bmatrix} S & 0 \\ 0 & S' \end{bmatrix}$$

Disconnected graphs

- Suppose graph is disconnected (still regular)

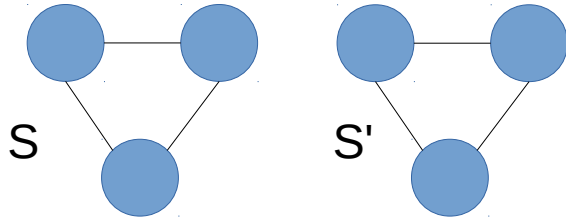


$$\text{Let } x_i^S = \begin{cases} 1 & \text{if } i \in S \\ 0 & \text{if } i \in S' \end{cases}$$

$$\begin{bmatrix} S & 0 \\ 0 & S' \end{bmatrix} \begin{bmatrix} 1 \\ \vdots \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = ?$$

Disconnected graphs

- Suppose graph is disconnected (still regular)



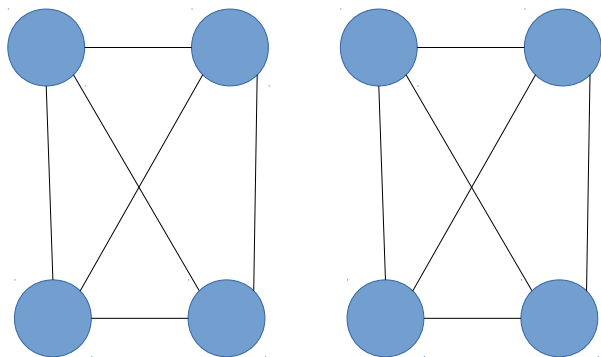
$$Ax^S = dx^S$$

$$Ax^{S'} = dx^{S'}$$

What happens if there are more than 2 connected components?

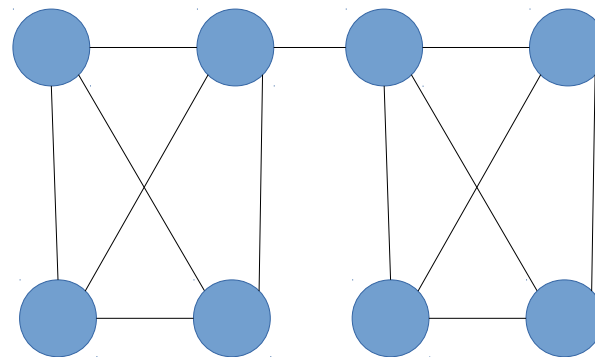
In general

Disconnected graph



$$\lambda_1 = \lambda_2$$

Almost disconnected graph



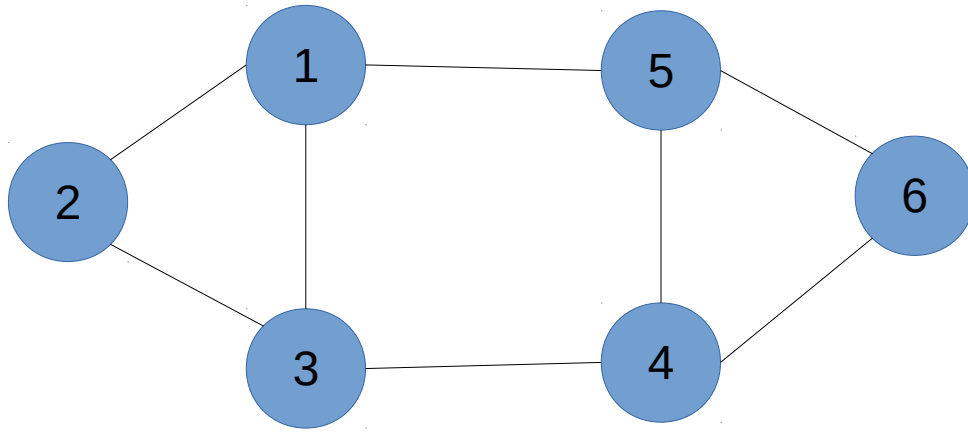
$$\lambda_1 \approx \lambda_2$$

Small “eigengap”

Graph Laplacian

Adjacency matrix

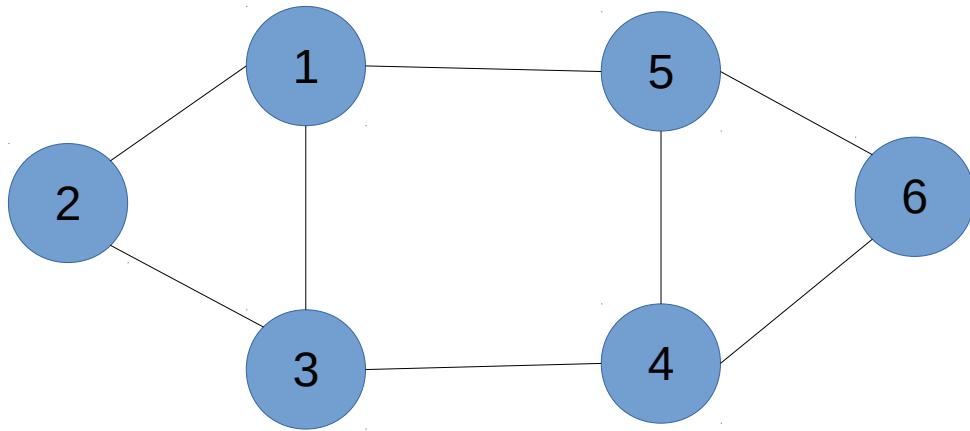
$$A_{ij} = \begin{cases} 1 & \text{if } (i, j) \in E \\ 0 & \text{otherwise} \end{cases}$$



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

Degree matrix

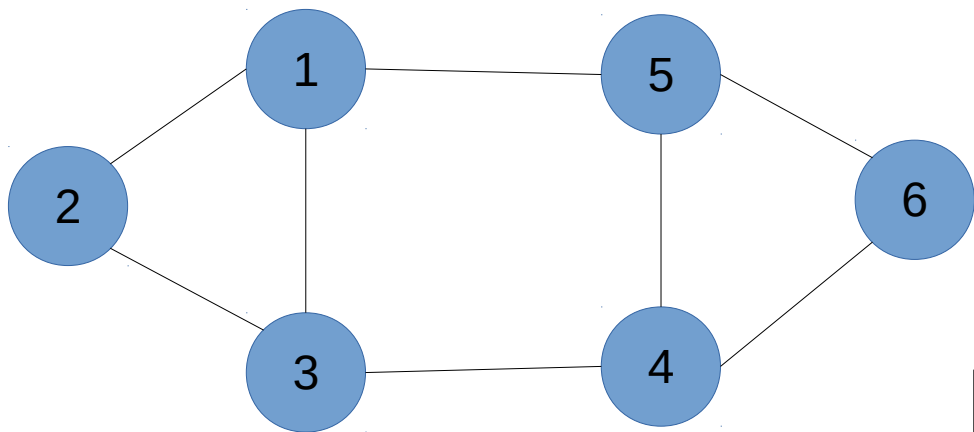
$$D_{ij} = \begin{cases} k_i & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$



$$D = \begin{bmatrix} 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix}$$

Laplacian matrix

$$L = D - A$$



$$L = \begin{bmatrix} 3 & -1 & -1 & 0 & -1 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 3 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ -1 & 0 & 0 & -1 & 3 & -1 \\ 0 & 0 & 0 & -1 & -1 & 2 \end{bmatrix}$$

Laplacian matrix $L = D - A$

- Symmetric
- Eigenvalues non-negative and real
- Eigenvectors real and orthogonal

$$L\vec{1} = \begin{bmatrix} 3 & -1 & -1 & 0 & -1 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 3 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ -1 & 0 & 0 & -1 & 3 & -1 \\ 0 & 0 & 0 & -1 & -1 & 2 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = ?$$

Constant vector is eigenvector of L

- The constant vector $x=[1,1,\dots,1]^T$ is an eigenvector, and has eigenvalue 0

$$Lx = \begin{bmatrix} 3 & -1 & -1 & 0 & -1 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 3 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ -1 & 0 & 0 & -1 & 3 & -1 \\ 0 & 0 & 0 & -1 & -1 & 2 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = 0 \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

- Is this true **for this graph** or **for any graph**?

If the graph is disconnected

- If there are two connected components, the same argument as for the adjacency matrix applies, and $\lambda_1 = \lambda_2 = 0$
- The multiplicity of eigenvalue 0 is equal to the number of connected components

$$x^T L x$$

Prove this!

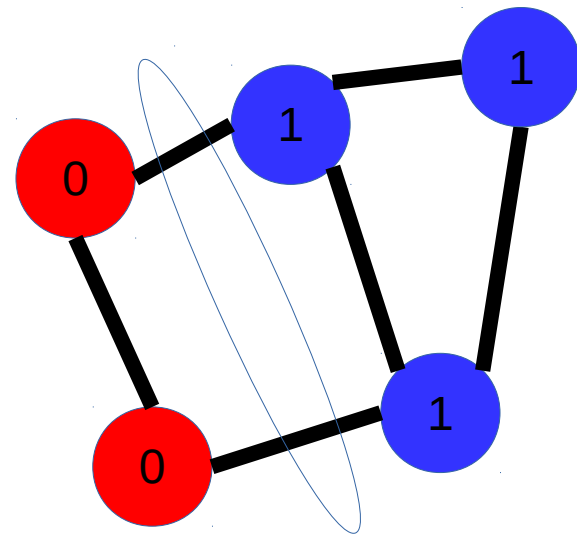
- Prove that $\sum_{(i,j) \in E} (x_i - x_j)^2 = x^T L x$

$$L = D - A$$

$$D_{ij} = \begin{cases} k_i & \text{if } i = j \\ 0 & \text{otherwise} \end{cases} \quad A_{ij} = \begin{cases} 1 & \text{if } (i, j) \in E \\ 0 & \text{otherwise} \end{cases}$$

$x^T L x$ and graph cuts

- Suppose (S, S') is a cut of graph G
- Set $x_i = \begin{cases} 1 & \text{if } i \in S \\ 0 & \text{if } i \in S' \end{cases}$



$$|c(S, S')| = 2$$

$$x^T L x = \sum_{(i,j) \in E} (x_i - x_j)^2 = \sum_{(i,j) \in c(S, S')} 1^2 = |c(S, S')|$$

Important fact

- For symmetric matrices

$$\lambda_2 = \min_x \frac{x^T M x}{x^T x}$$

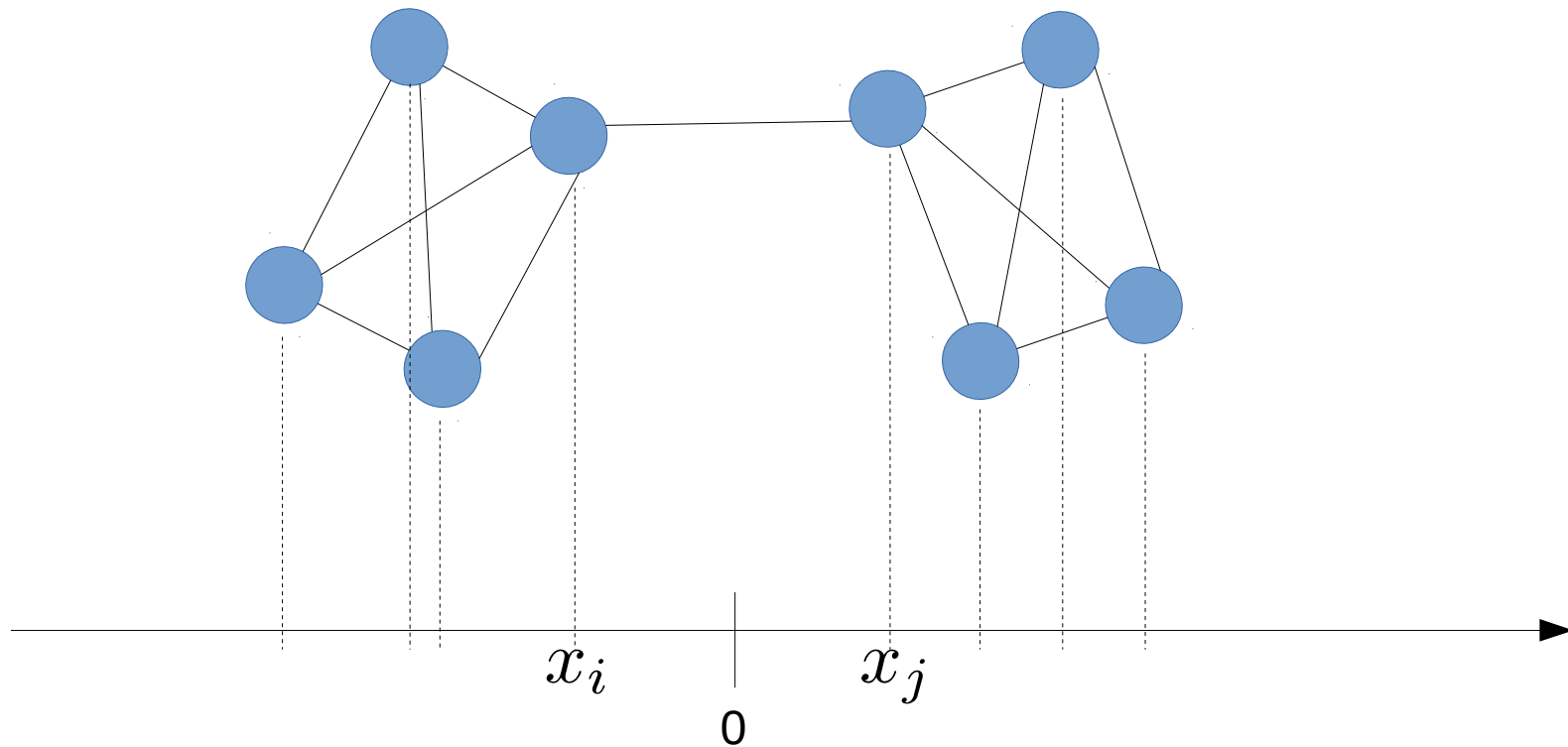
Second eigenvector

- Orthogonal to the first one: $x \cdot \vec{1} = 0 \Rightarrow \sum_i x_i = 0$
- Normal: $\sum_i x_i^2 = 1$

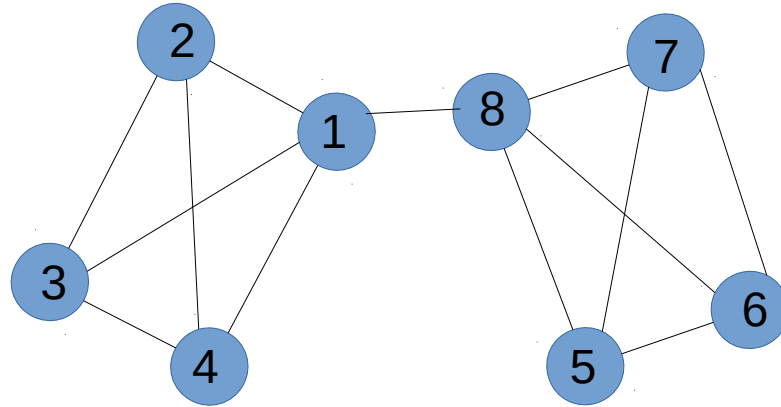
$$\lambda_2 = \min_x \frac{x^T L x}{x^T x} = \min_{x: \sum x_i = 0} \frac{x^T L x}{\sum x_i^2} = \min_{x: \sum x_i = 0} \sum_{(i,j) \in E} (x_i - x_j)^2$$

What does this mean?

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

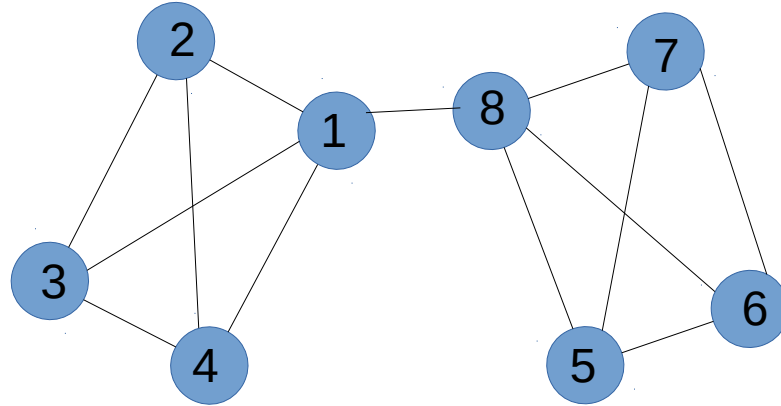


Example Graph 1



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

Example Graph 1 (second eigenvalue)



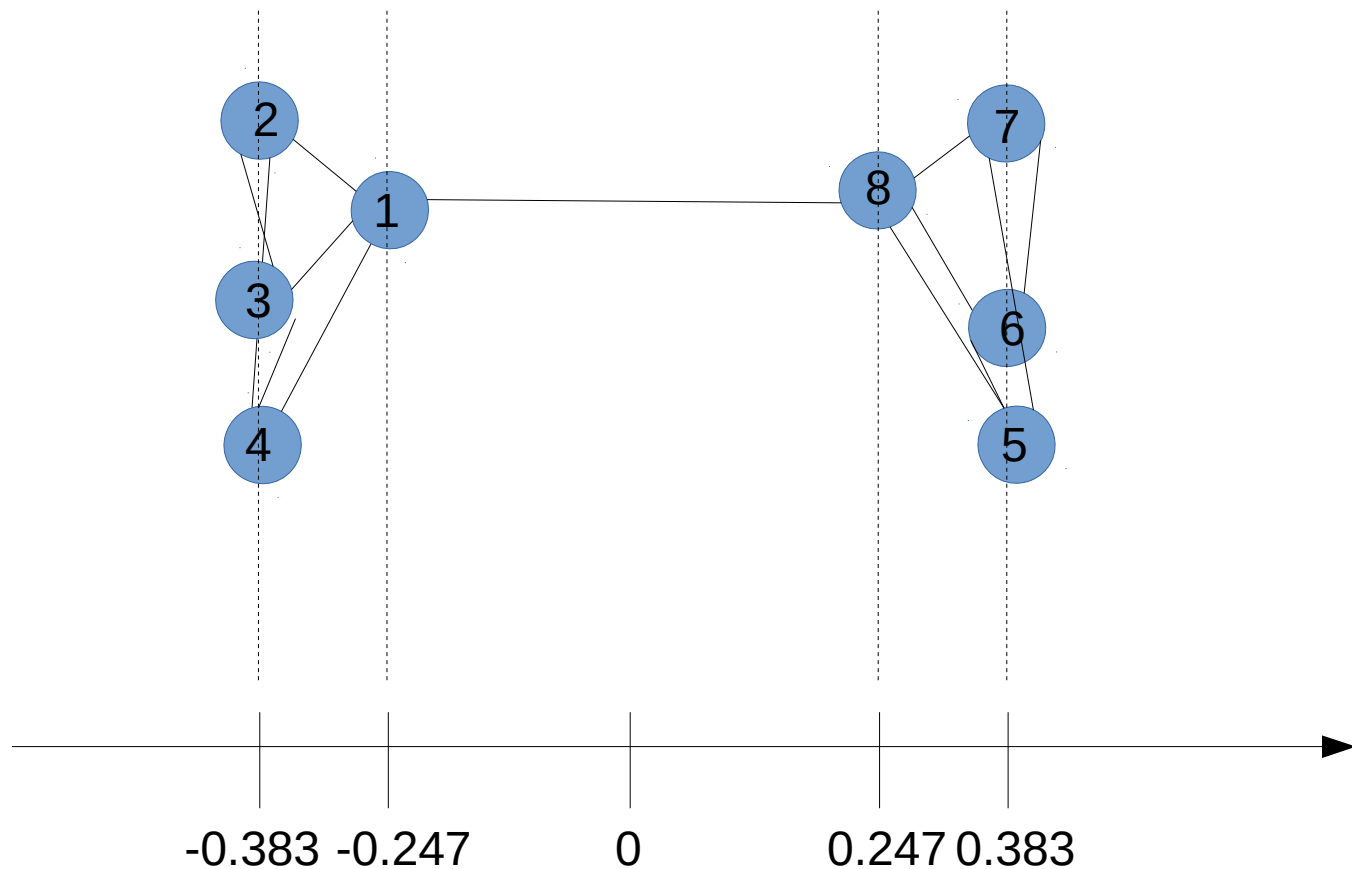
$$\lambda_1 = 0$$

$$\lambda_2 = 0.354$$

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

$$v_2 = \begin{bmatrix} 0.247 \\ 0.383 \\ 0.383 \\ 0.383 \\ -0.383 \\ -0.383 \\ -0.383 \\ -0.247 \end{bmatrix}$$

Example Graph 1, projected

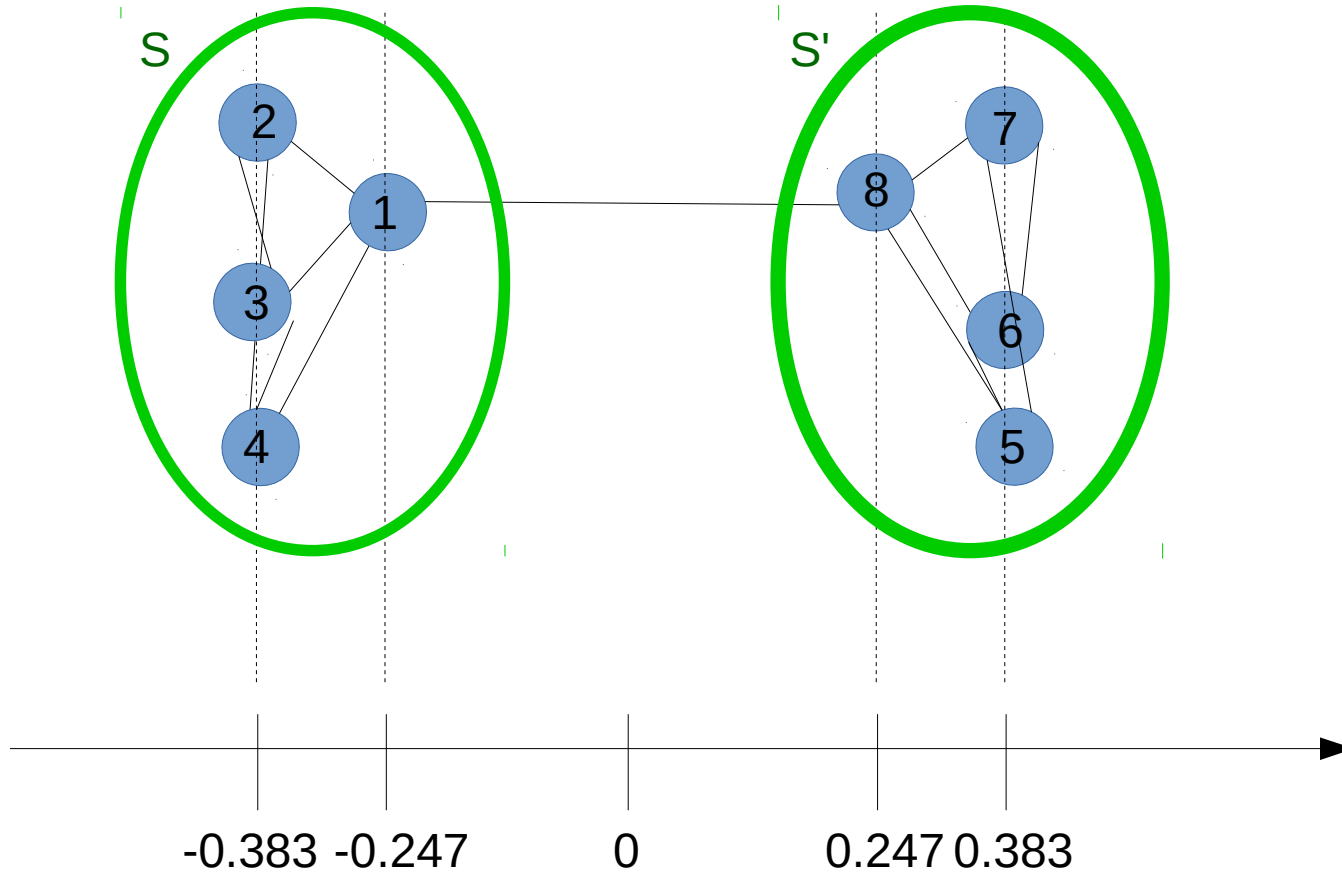


$$\lambda_1 = 0$$

$$\lambda_2 = 0.354$$

$$v_2 = \begin{bmatrix} 0.247 \\ 0.383 \\ 0.383 \\ 0.383 \\ -0.383 \\ -0.383 \\ -0.383 \\ -0.247 \end{bmatrix}$$

Example Graph 1, communities

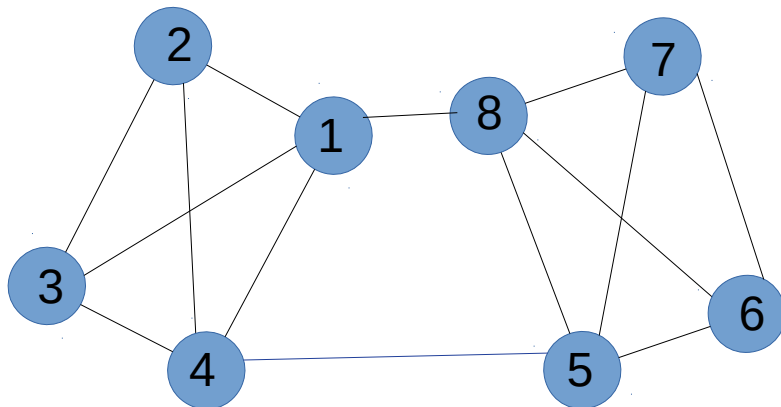


$$\lambda_1 = 0$$

$$\lambda_2 = 0.354$$

$$v_2 = \begin{bmatrix} 0.247 \\ 0.383 \\ 0.383 \\ 0.383 \\ -0.383 \\ -0.383 \\ -0.383 \\ -0.247 \end{bmatrix}$$

Example Graph 2



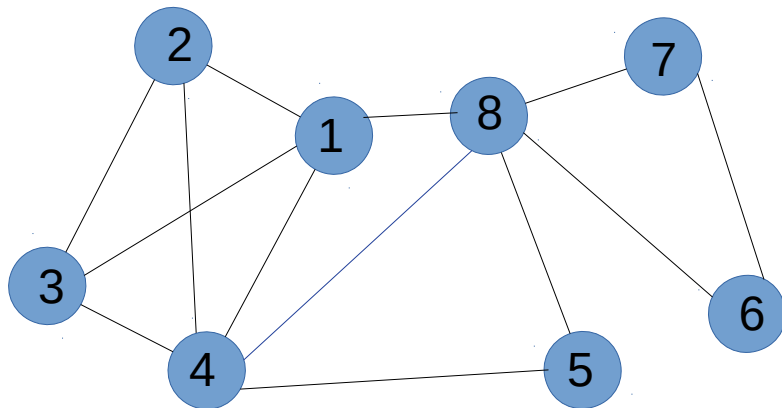
$$\lambda_1 = 0$$

$$\lambda_2 = 0.764$$

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

$$v_2 = \begin{bmatrix} 0.263 \\ 0.425 \\ 0.425 \\ 0.263 \\ -0.263 \\ -0.425 \\ -0.425 \\ -0.263 \end{bmatrix}$$

Example Graph 3



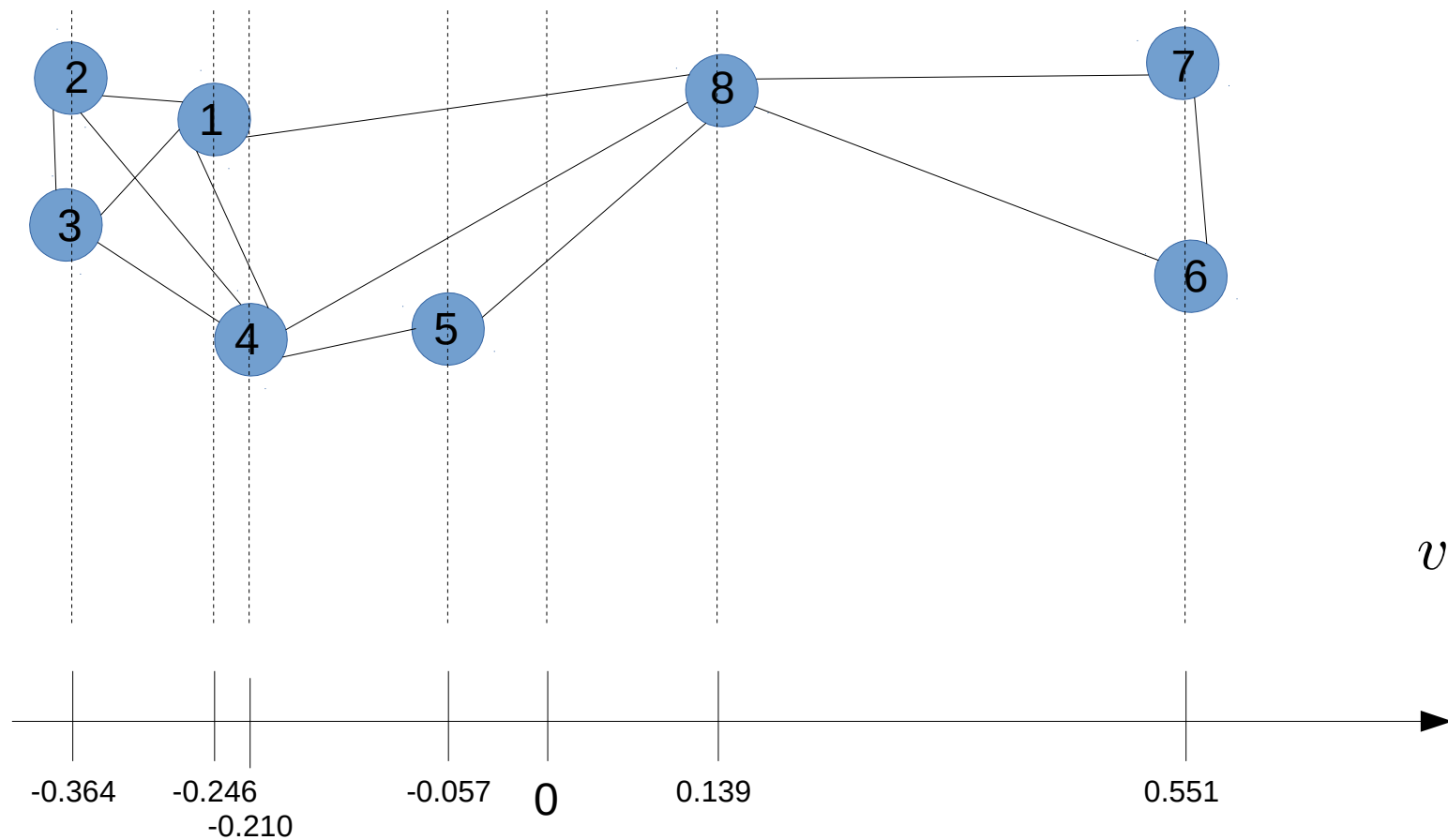
$$\lambda_1 = 0$$

$$\lambda_2 = 0.748$$

$$L = \begin{bmatrix} 4 & -1 & -1 & -1 & 0 & 0 & 0 & -1 \\ -1 & 3 & -1 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 3 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & -1 & 5 & -1 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 2 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 2 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 \\ -1 & 0 & 0 & -1 & -1 & -1 & -1 & 5 \end{bmatrix}$$

$$v_2 = \begin{bmatrix} -0.246 \\ -0.364 \\ -0.364 \\ -0.210 \\ -0.057 \\ 0.551 \\ 0.551 \\ 0.139 \end{bmatrix}$$

Example Graph 3, projected (where to cut?)

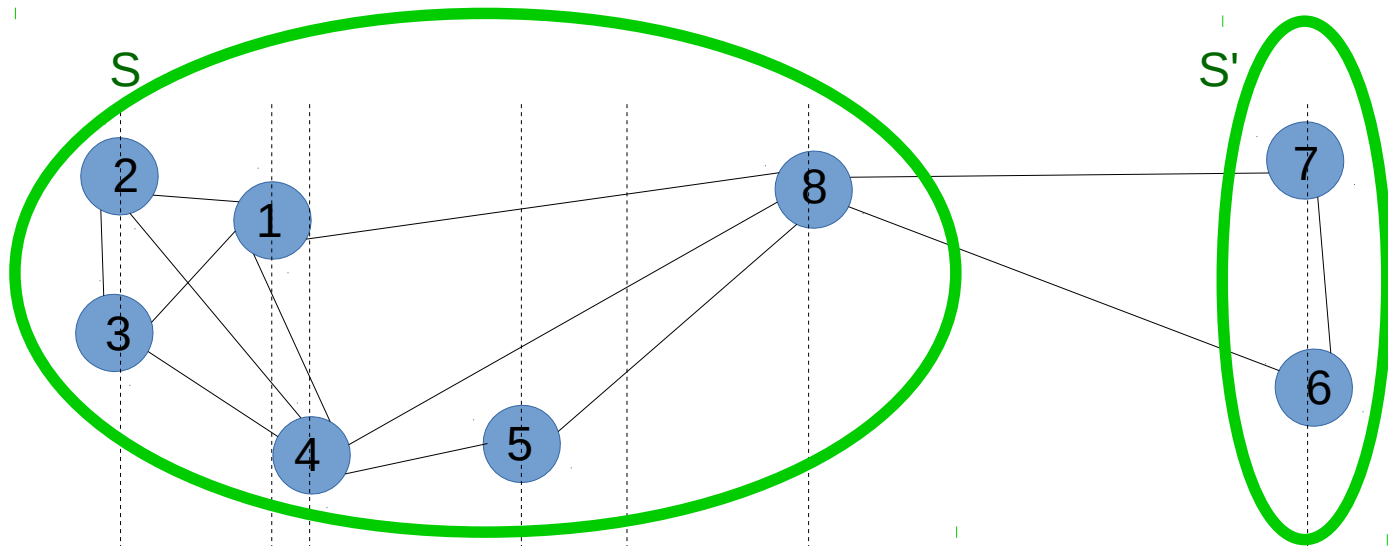


$$\lambda_1 = 0$$

$$\lambda_2 = 0.748$$

$$v_2 = \begin{bmatrix} -0.246 \\ -0.364 \\ -0.364 \\ -0.210 \\ -0.057 \\ 0.551 \\ 0.551 \\ 0.139 \end{bmatrix}$$

Example Graph 3, projected (where to cut?)



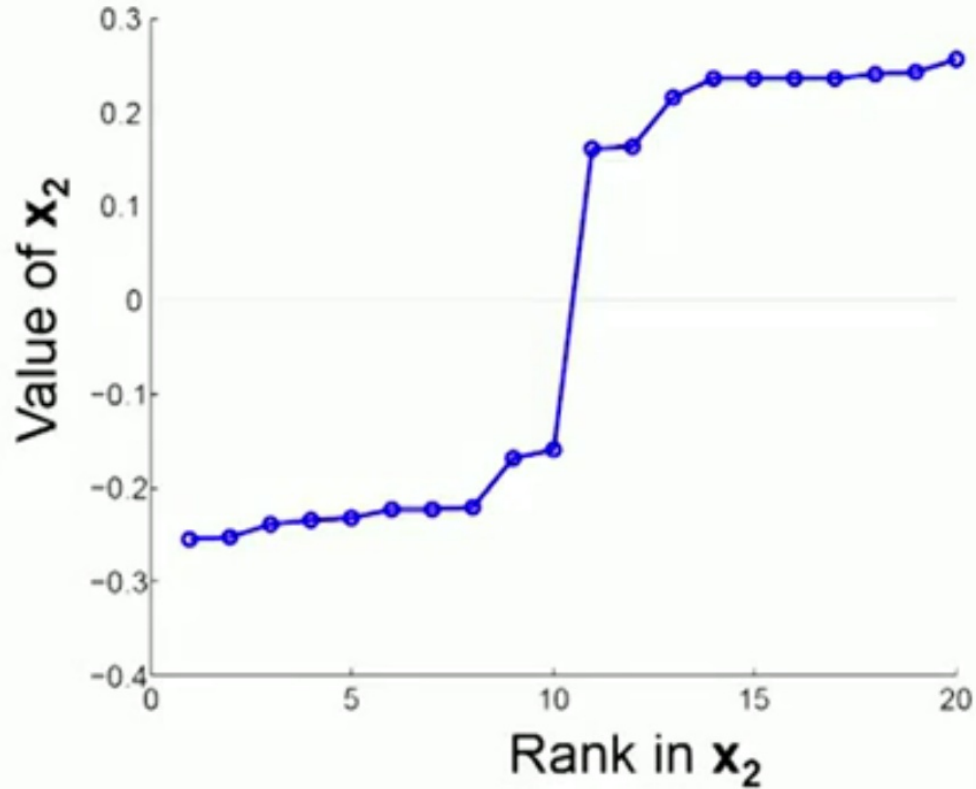
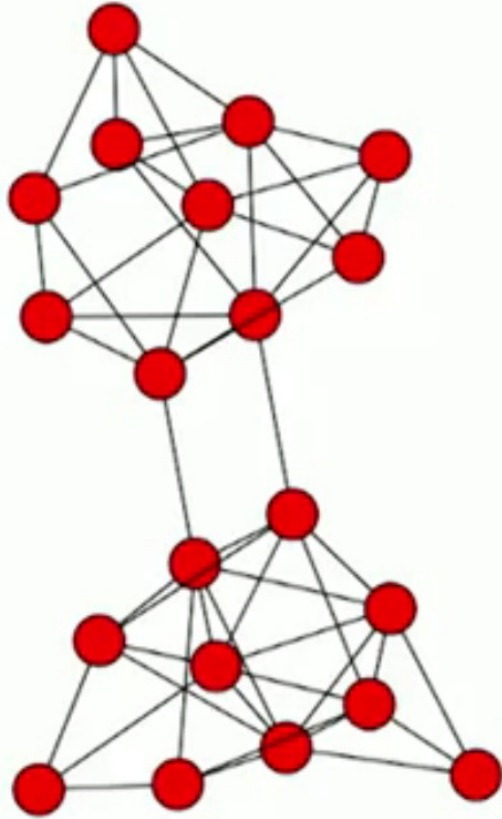
$$\lambda_1 = 0$$

$$\lambda_2 = 0.748$$

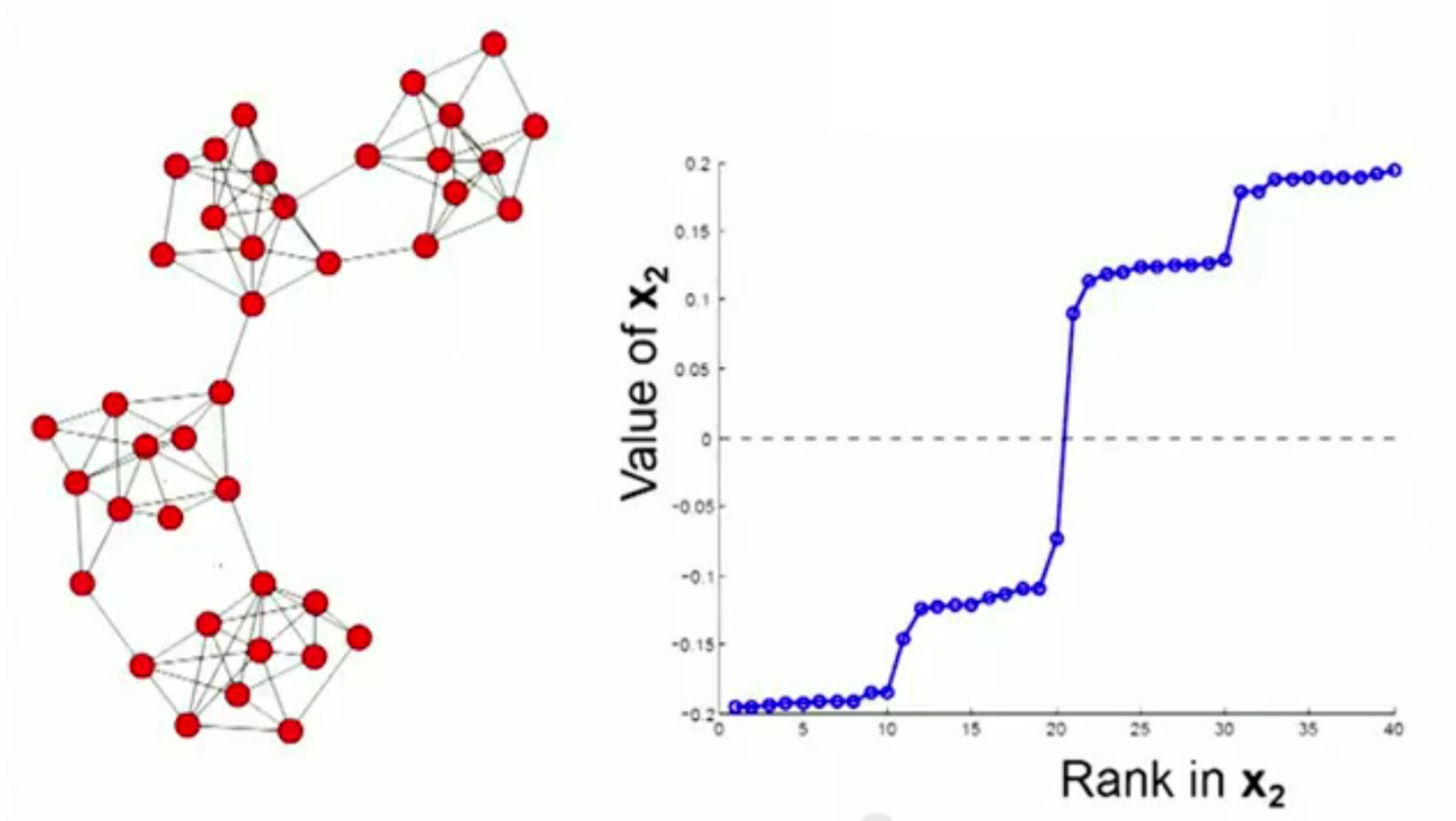
$$v_2 =$$

$$\begin{bmatrix} -0.246 \\ -0.364 \\ -0.364 \\ -0.210 \\ -0.057 \\ 0.551 \\ 0.551 \\ 0.139 \end{bmatrix}$$

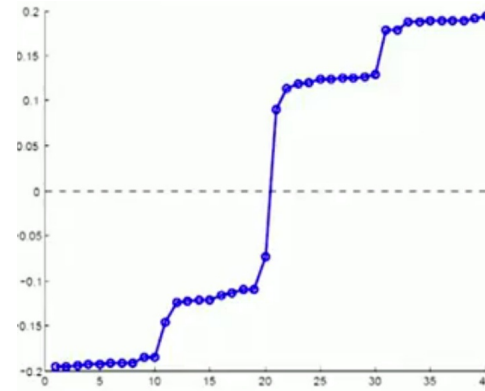
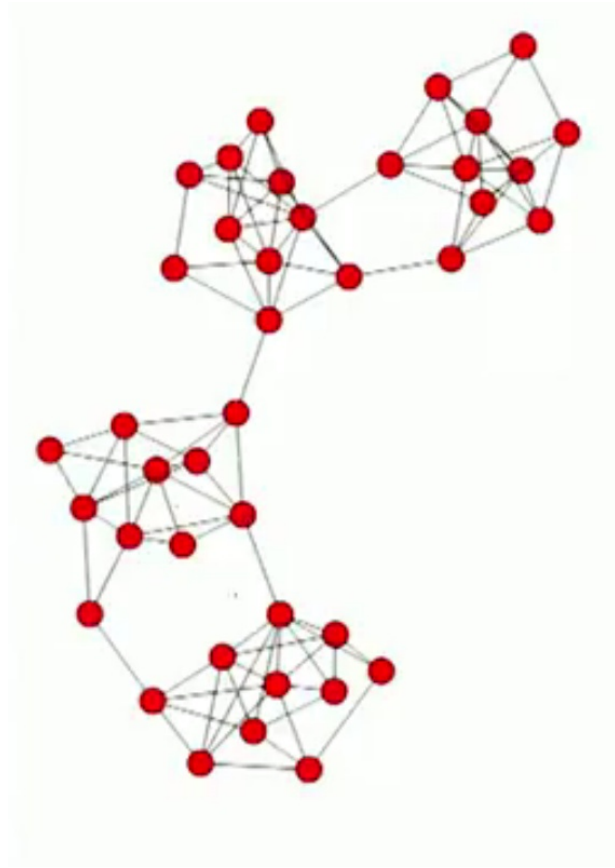
A more complex graph



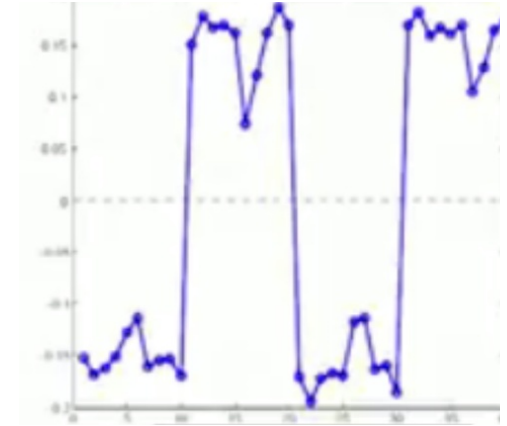
A graph with 4 “communities”



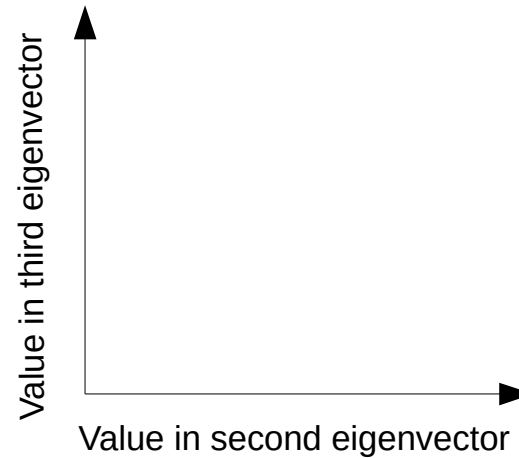
Other eigenvectors



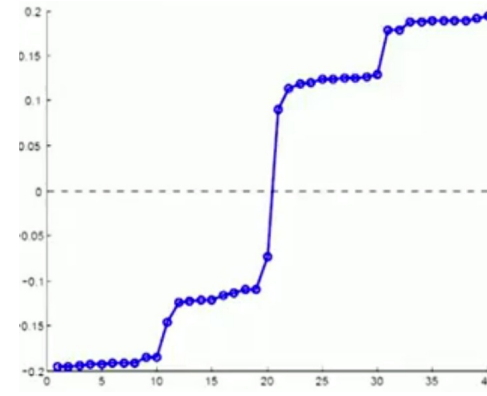
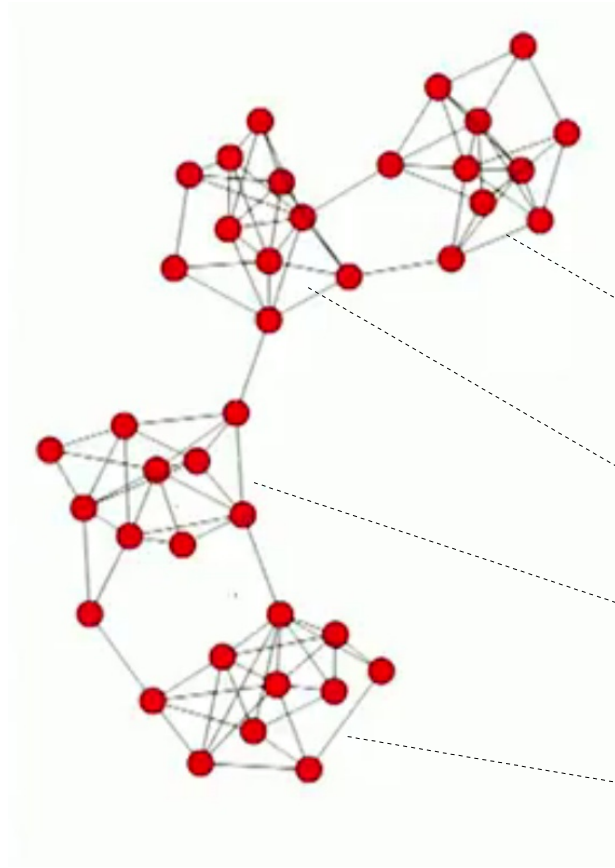
Second eigenvector



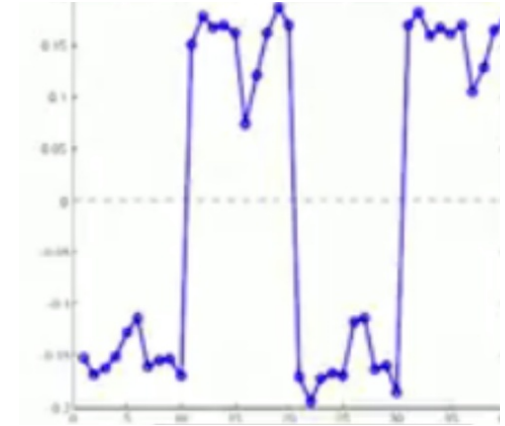
Third eigenvector



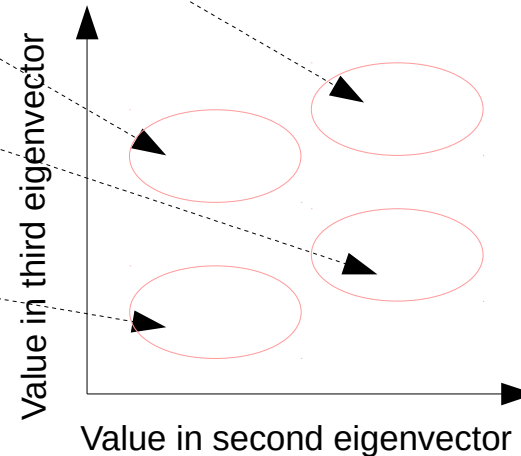
Other eigenvectors



Second eigenvector



Third eigenvector

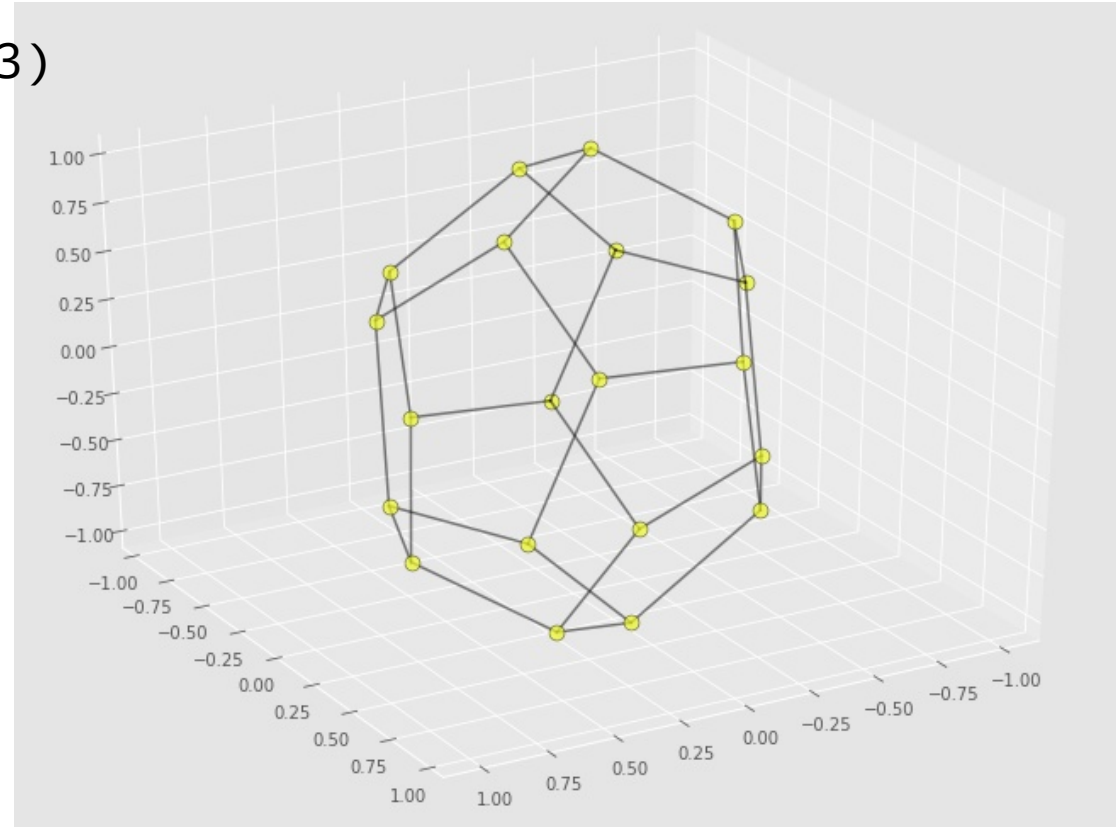


Clustering can be done using Euclidean distance

Dodecahedral graph in 3D

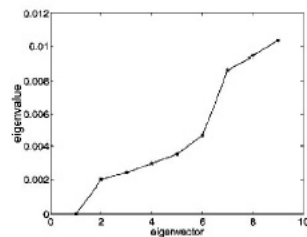


```
g = nx.dodecahedral_graph()  
pos = nx.spectral_layout(g, dim=3)  
network_plot_3D_alt(g, 60, pos)
```

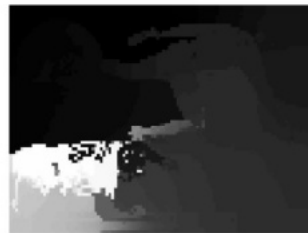


Application: image segmentation

[Shi & Malik 2000]



(a)



(b)



(c)

Transform into
grid graph with
edge weights
proportional to
pixel similarity



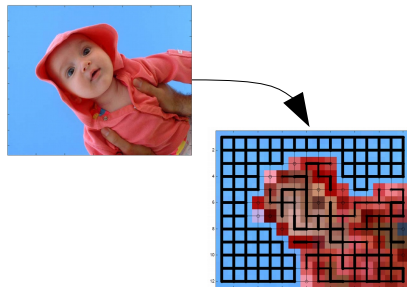
(d)



(e)



(f)



(g)



(h)



(i)

Summary

Things to remember

- Graph Laplacian
- Laplacian and graph components
- Spectral graph embedding

Exercises for this topic

- Mining of Massive Datasets (2014) by Leskovec et al.
 - Exercises 10.4.6