Spectral Graph Embedding

Social Networks Analysis and Graph Algorithms

Prof. Carlos Castillo — https://chato.cl/teach

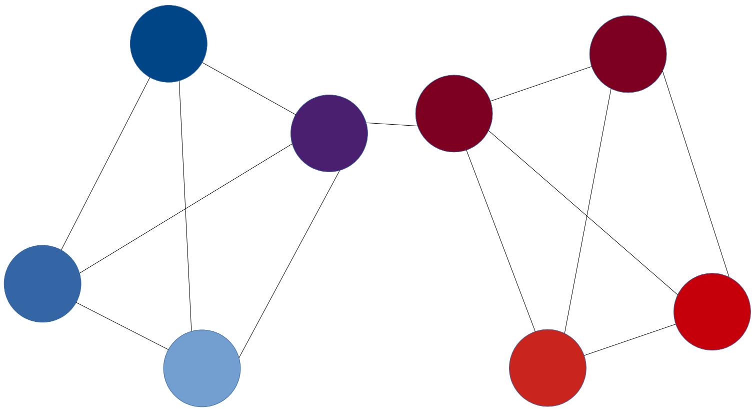
Universitat Pompeu Fabra Barcelona

Sources

- **J. Leskovec (2016). Defining the graph laplacian** [video]
- E. Terzi (2013). Graph cuts — The part on spectral graph partitioning
- D. A. Spielman (2009): The Laplacian
- URLs cited in the footer of slides

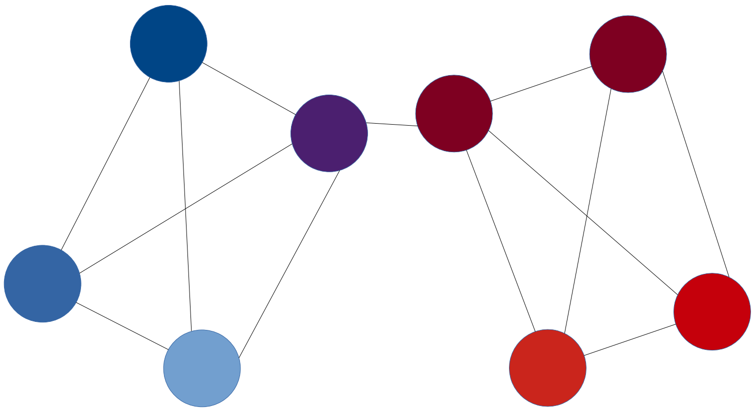
Graphs are nice, but ...

- They describe only local relationships
- We would like to understand a global structure
- We will try to transform a graph into a more familiar object: a cloud of points in R^k



Graphs are nice, but ...

- They describe only local relationships
- We would like to understand a global structure
- We will try to transform a graph into a more familiar object: a cloud of points in 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 on paper

Exercise: draw this graph

V = {v1, v2, ..., 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

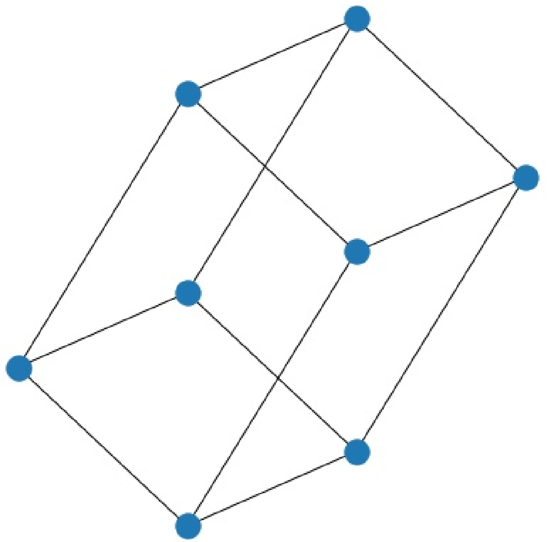
What constitutes a good drawing?

2D graph embeddings in NetworkX

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

G = nx.hypercube_graph(3)
display(list(G.edges()))
```

```
[((0, 0, 0), (1, 0, 0)),
 ((0, 0, 0), (0, 1, 0)),
 ((0, 0, 0), (0, 0, 1)),
 ((0, 0, 1), (1, 0, 1)),
 ((0, 0, 1), (0, 1, 1)),
 ((0, 1, 0), (1, 1, 0)),
 ((0, 1, 0), (0, 1, 1)),
 ((0, 1, 1), (1, 1, 1)),
 ((1, 0, 0), (1, 1, 0)),
 ((1, 0, 0), (1, 0, 1)),
 ((1, 0, 1), (1, 1, 1)),
 ((1, 1, 0), (1, 1, 1))]
```

```
plt.figure(figsize=(6,6))
nx.draw_spectral(G)
_ = plt.show()
```



In a good graph embedding ...

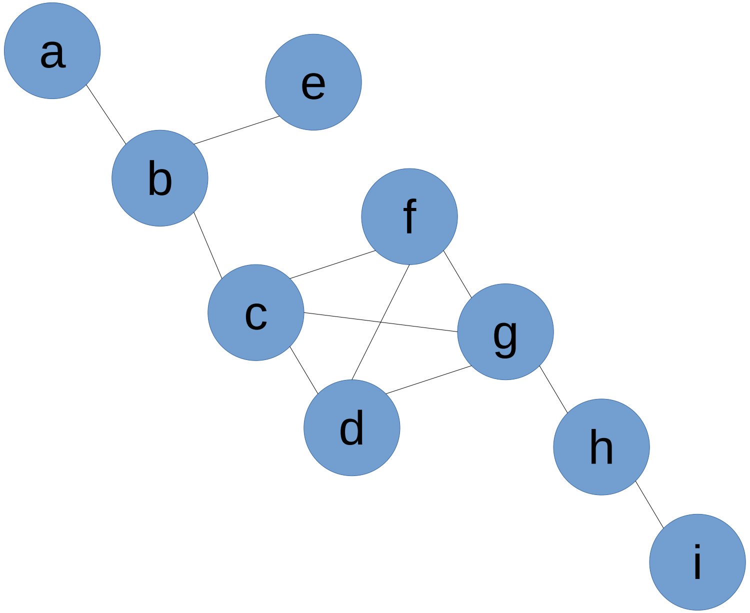
- Pairs of nodes that are **connected** to each other should be **close**
- Pairs of nodes that are not connected should be far
- Compromises will need to be made

Random graph projection (2D)

- 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)

Exercise: random projection

- Given this graph
- Pick a random node *u*
  - Distances from *u* are the x positions
- Pick a random node v
  - Distances from *v* are the y positions
- Draw the graph in an R^2 plane



Eigenvectors of the adjacency matrix

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?

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

https://www.youtube.com/watch?v=AR7iFxM-NkA

Adjacency matrix of G=(V,E)

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

What is y_i?

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

https://www.youtube.com/watch?v=AR7iFxM-NkA

Adjacency matrix of G=(V,E)

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

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

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

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

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

https://www.youtube.com/watch?v=AR7iFxM-NkA

Spectral graph theory ...

- Studies 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?

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

An eigenvector of a d-regular graph

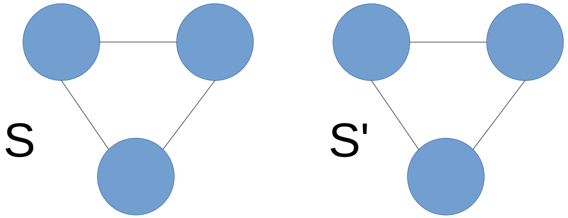
- Suppose graph is d-regular, i.e. all nodes have degree d:

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

- **Hence, $[1, 1, \ldots, 1]^T$ is an eigenvector of eigenvalue d**

Disconnected graphs

- Suppose the graph is regular **and disconnected**

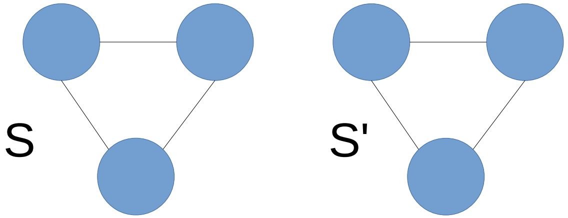


- Then its adjacency matrix has block structure:

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

Disconnected graphs

- Suppose the graph is regular **and disconnected**

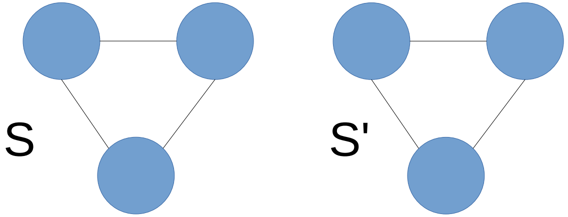


$$\text{Let } x_i^S = \begin{cases} 1 & \text{if } i \in S \\ 0 & \text{if } i \in S' \end{cases}$$

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

Disconnected graphs

- Suppose the graph is regular **and disconnected**

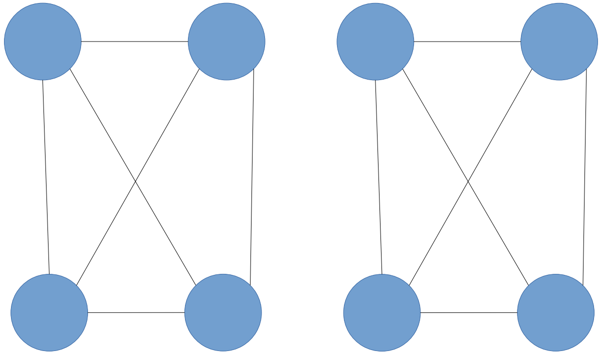
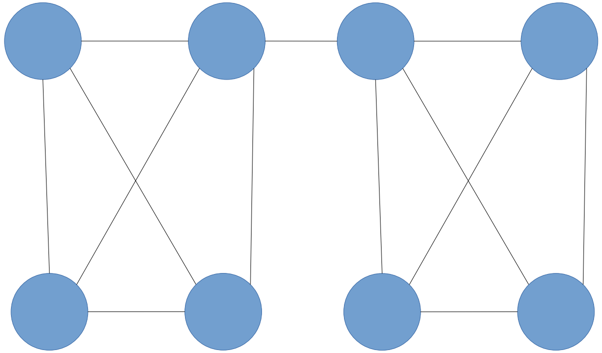


$$Ax^S = dx^S$$

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

- What is the multiplicity of eigenvalue d?
- What happens if there are more than 2 connected components?

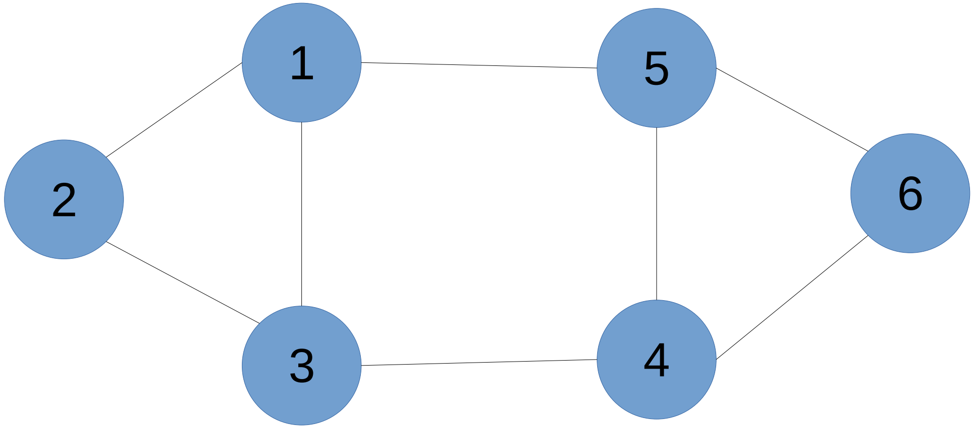
In general

Disconnected graph	*Almost* disconnected graph
	
$\lambda_1 = \lambda_2$	$\lambda_1 \approx \lambda_2$
	Small “**eigengap**”

Graph Laplacian

Adjacency matrix

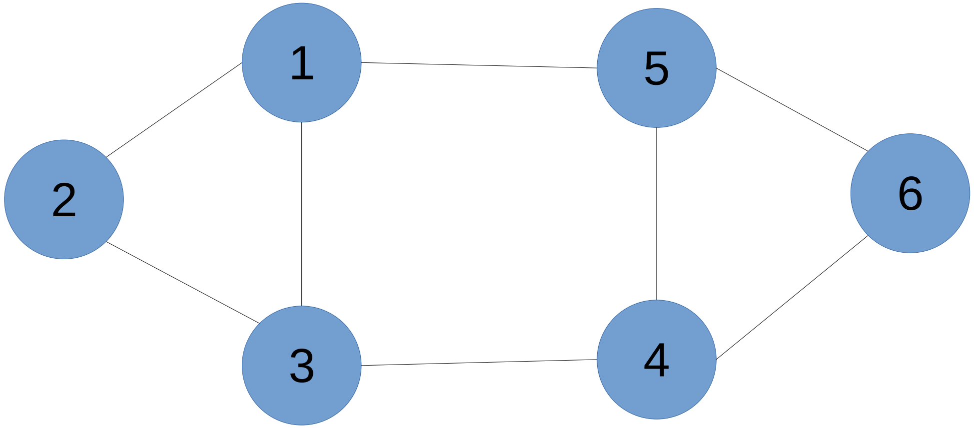
$$A_{ij} = \begin{cases} 1 & \text{if } (i,j) \in E \\ 0 & \text{otherwise} \end{cases}$$



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

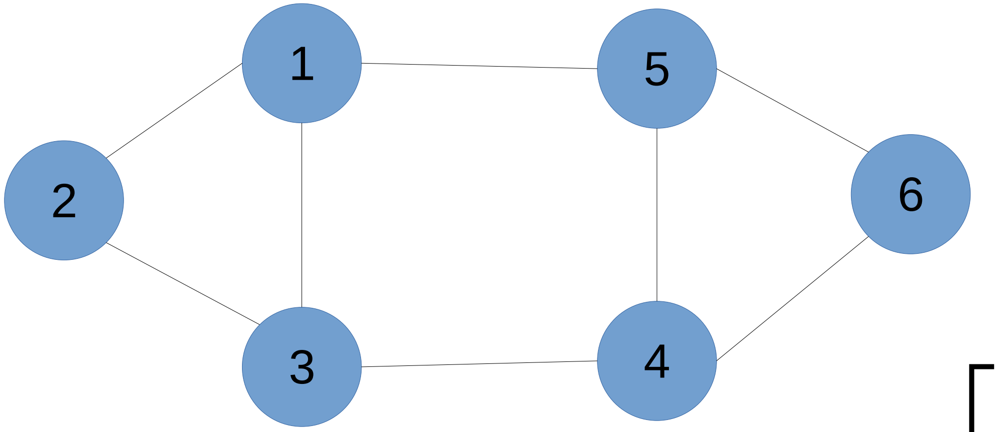
Degree matrix

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



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

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=$[1,1,\ldots,1]^\top$ 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 the graph is disconnected into two 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 $\sum_{(i,j)\in E}(x_i - x_j)^2 = x^T L x$

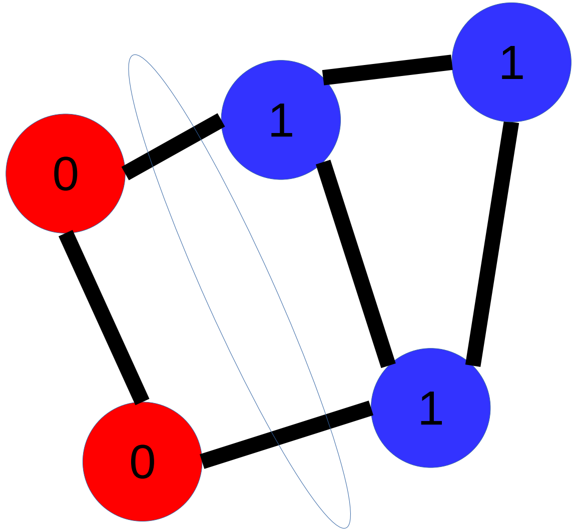
$$L = D - A$$

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

Think of this quantity as the “stress” produced by the assignment of node labels x

$x^T Lx$ and graph cuts

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



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

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

Important fact

- For symmetric matrices

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

https://en.wikipedia.org/wiki/Rayleigh_quotient

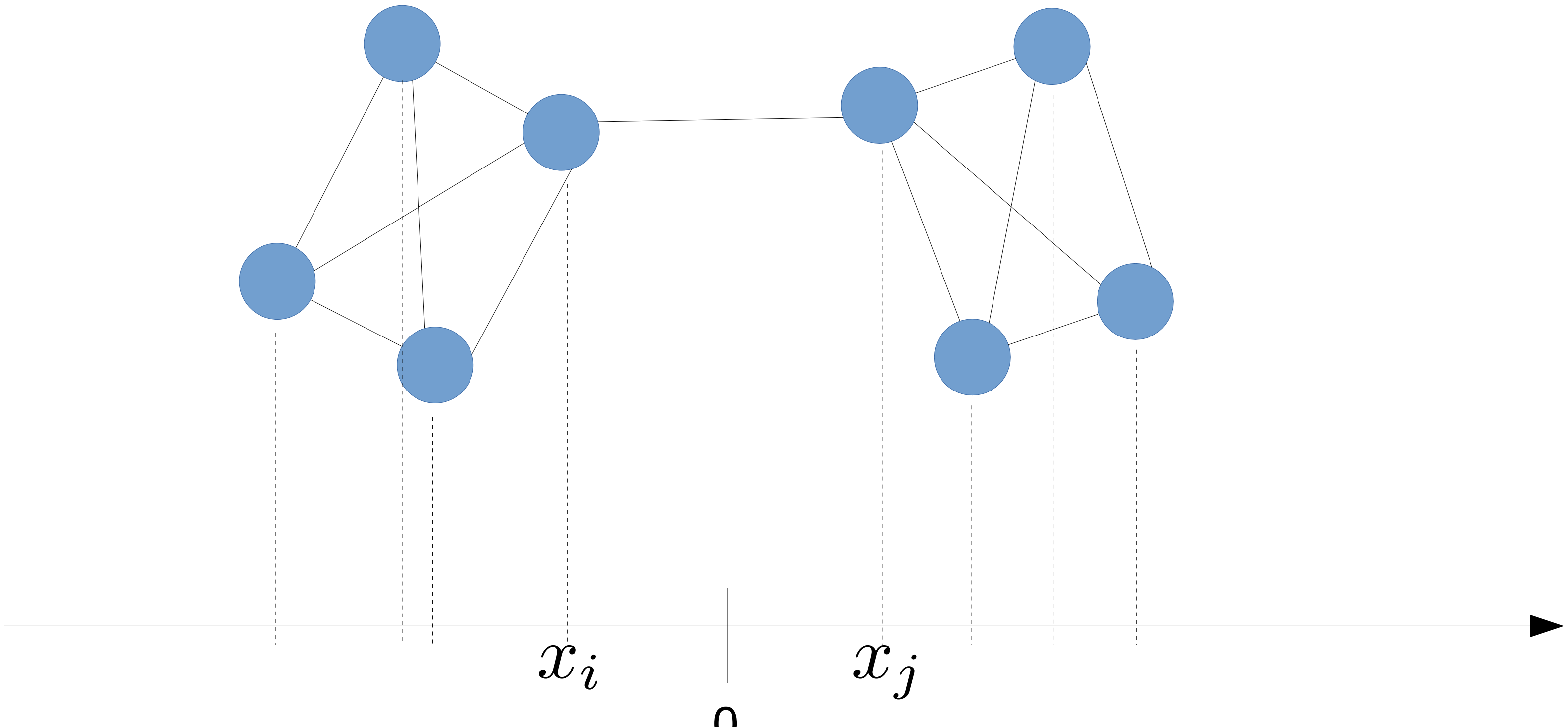
Second eigenvector

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

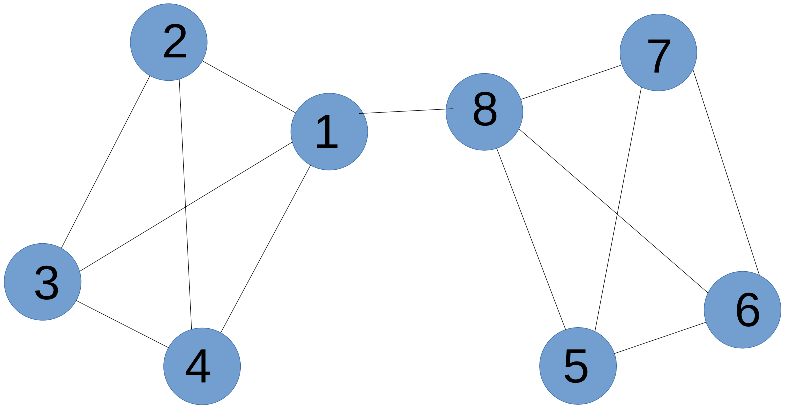
$$\lambda_2 = \min_x \frac{x^T L x}{x^T x} = \min_{x:\sum x_i = 0} \frac{x^T L x}{\sum x_i^2} = \min_{x:\sum x_i = 0} \sum_{(i,j) \in E} (x_i - x_j)^2$$

What does this mean?

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

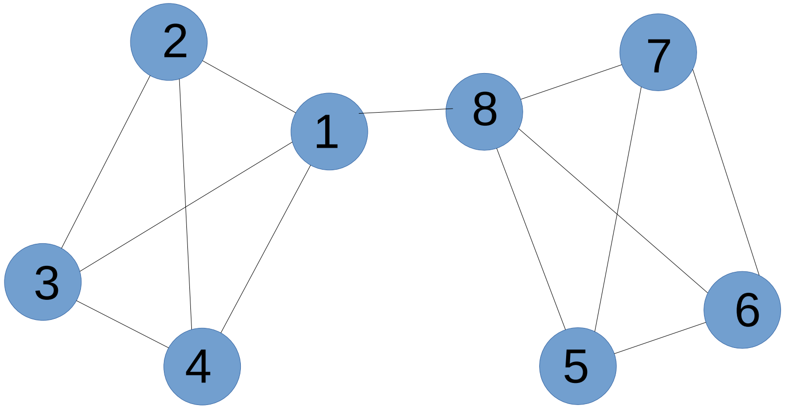


Example Graph 1



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

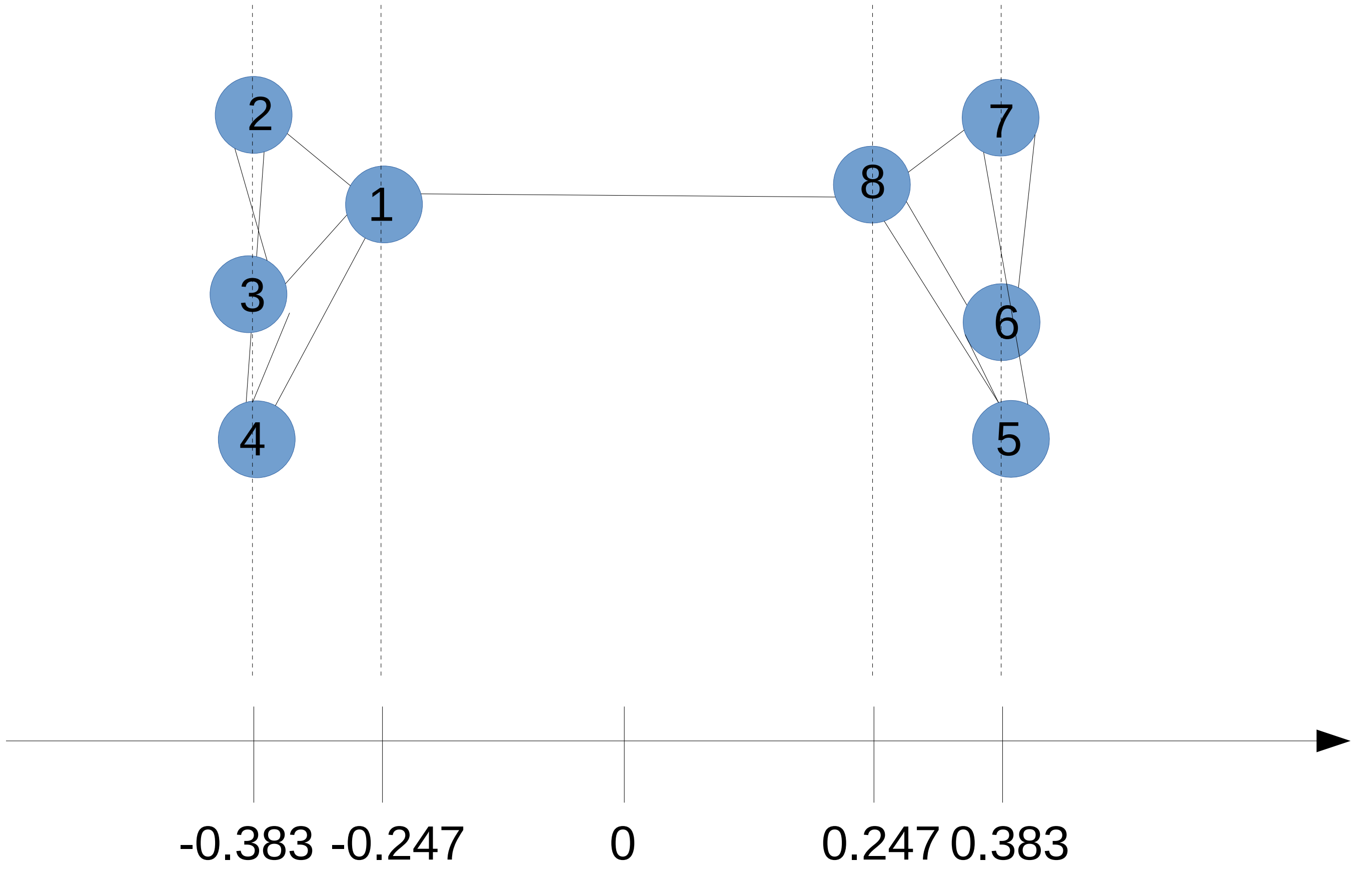
Example Graph 1 (second eigenvalue)



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

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

Example Graph 1, projected in R^1

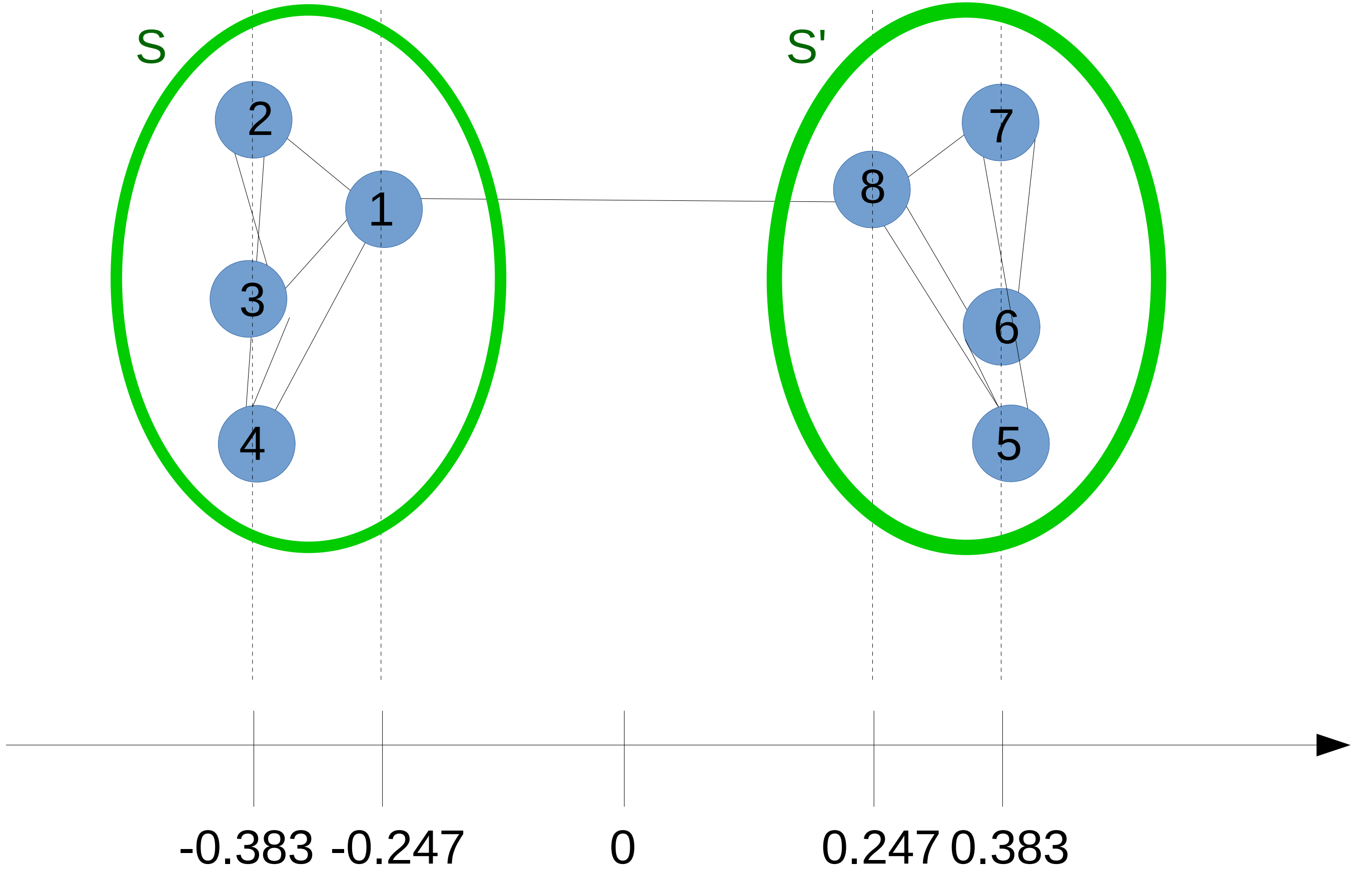


$$\lambda_1 = 0$$

$$\lambda_2 = 0.354$$

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

Example Graph 1, communities

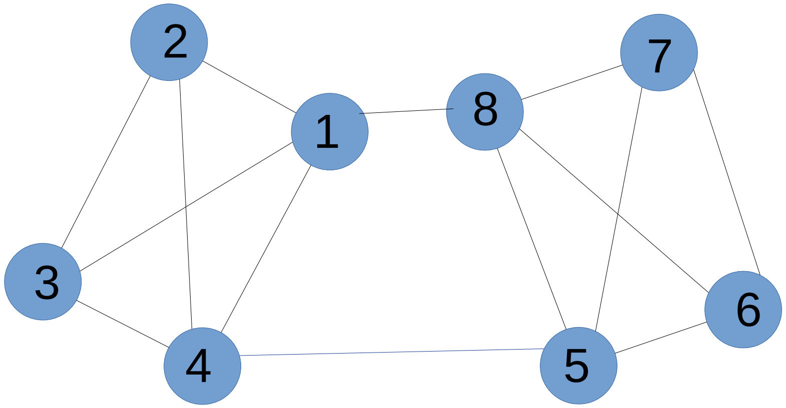


$$\lambda_1 = 0$$

$$\lambda_2 = 0.354$$

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

Example Graph 2



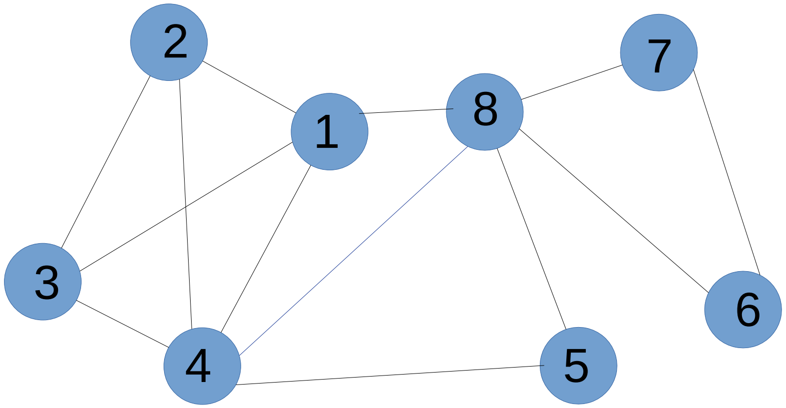
$$\lambda_1 = 0$$

$$\lambda_2 = 0.764$$

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

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

Example Graph 3



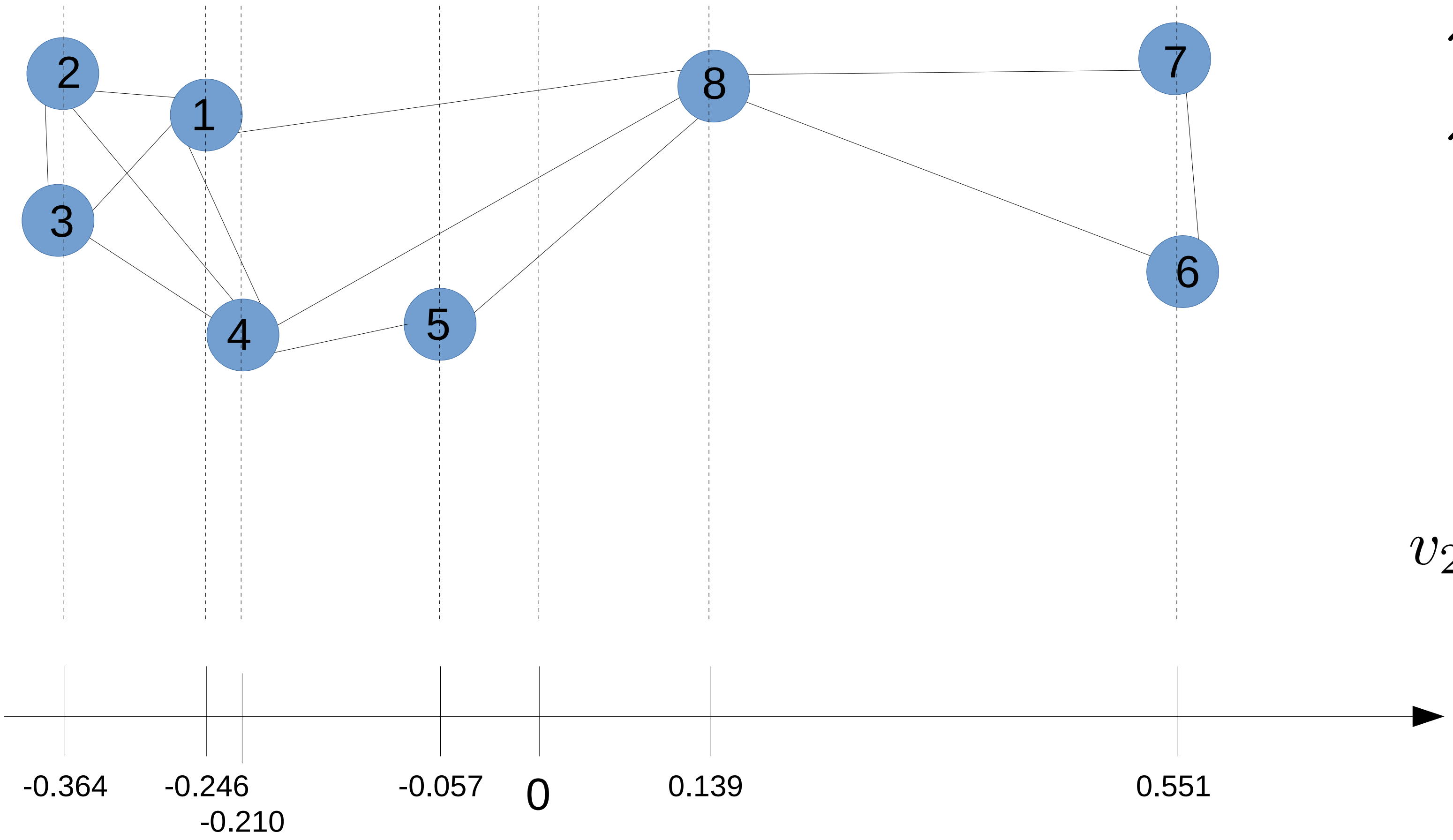
$$\lambda_1 = 0$$

$$\lambda_2 = 0.748$$

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

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

Example Graph 3, projected (where to cut?)

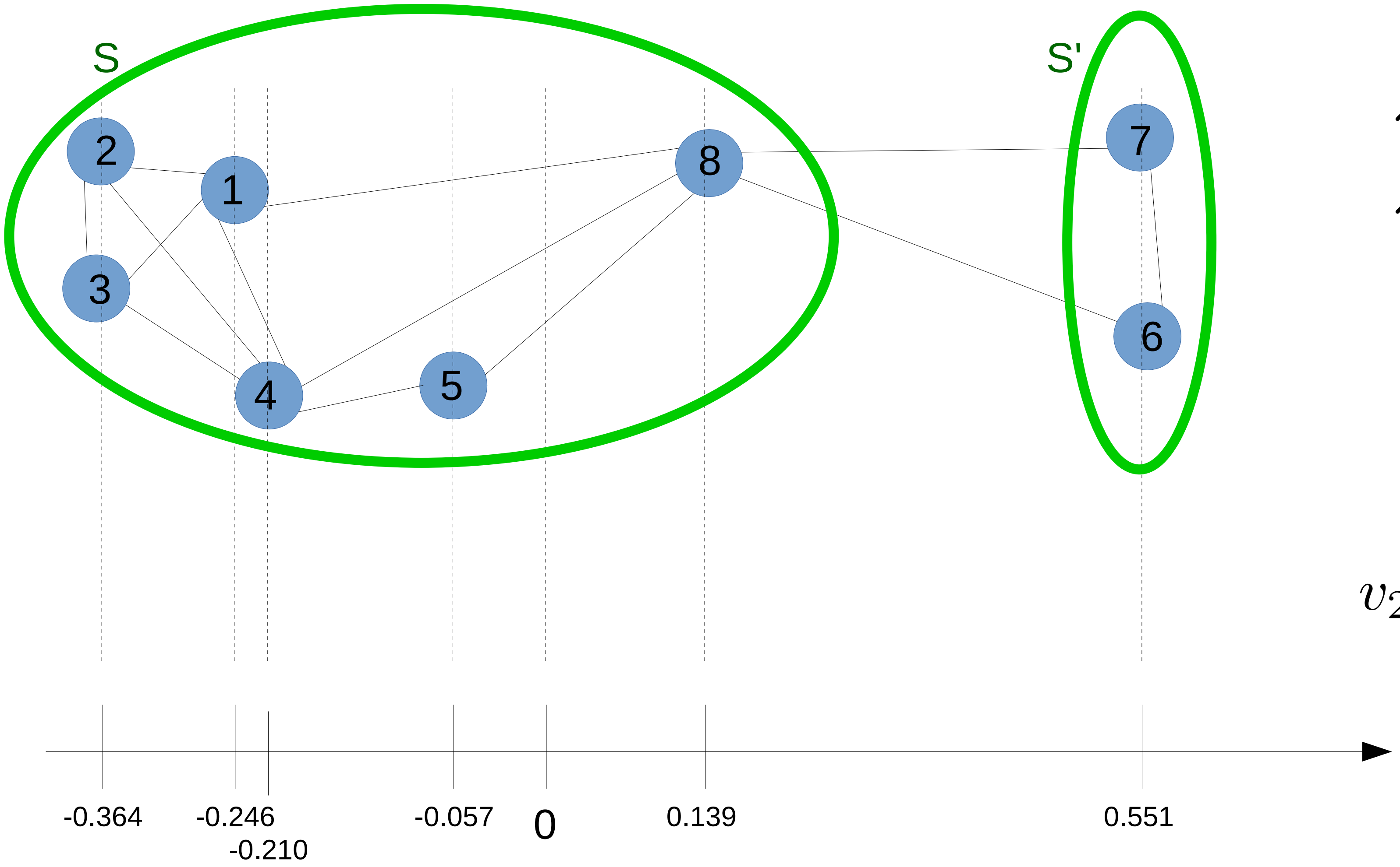


$$\lambda_1 = 0$$

$$\lambda_2 = 0.748$$

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

Example Graph 3, projected (where to cut?)

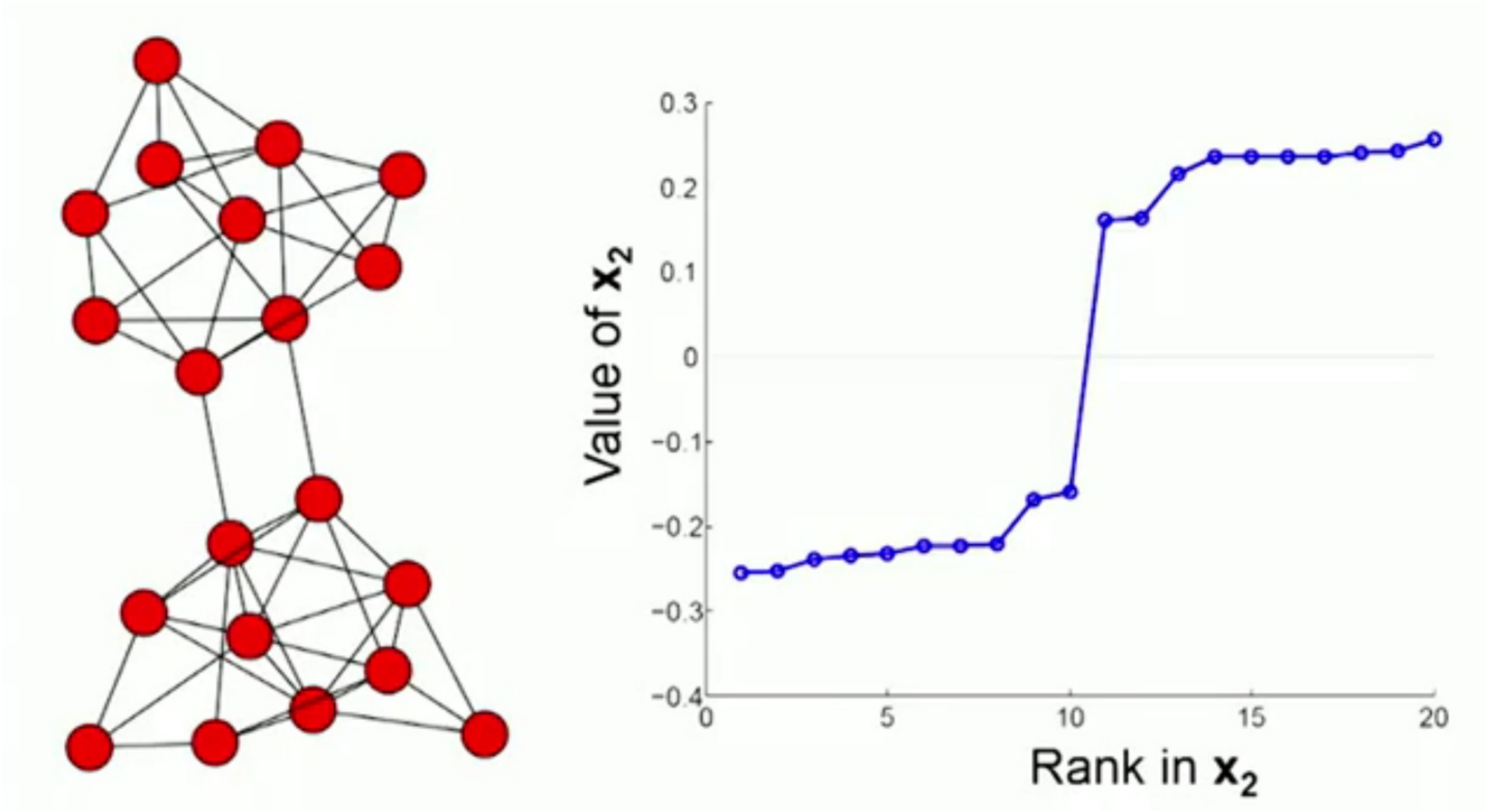


$$\lambda_1 = 0$$

$$\lambda_2 = 0.748$$

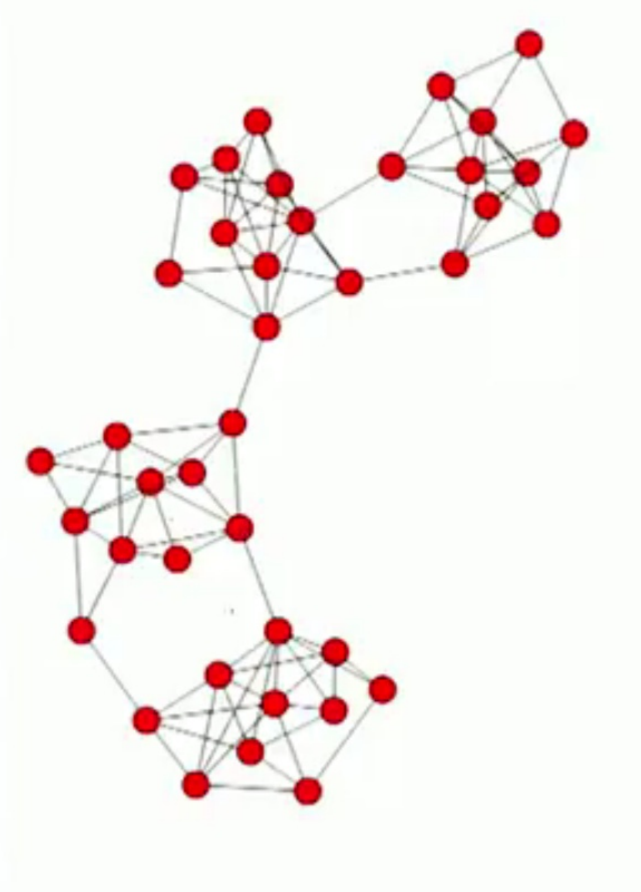
$$v_2 = \begin{bmatrix} -0.246 \\ -0.364 \\ -0.364 \\ -0.210 \\ -0.057 \\ 0.551 \\ 0.551 \\ 0.139 \end{bmatrix}$$

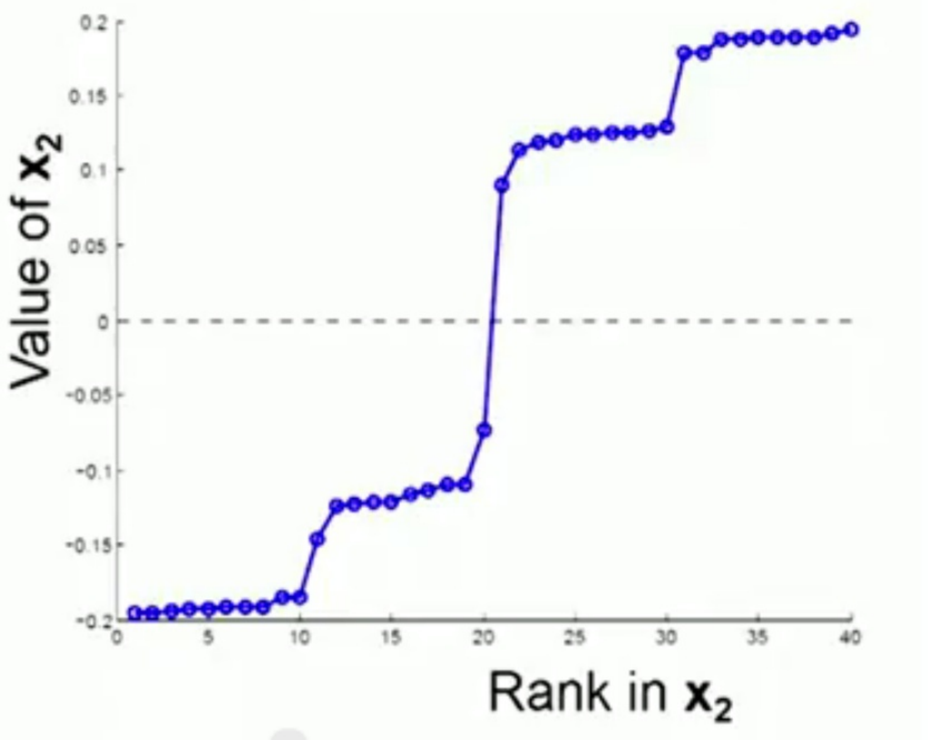
A graph with two communities in R^1



https://www.youtube.com/watch?v=jpTjj5PmcMM

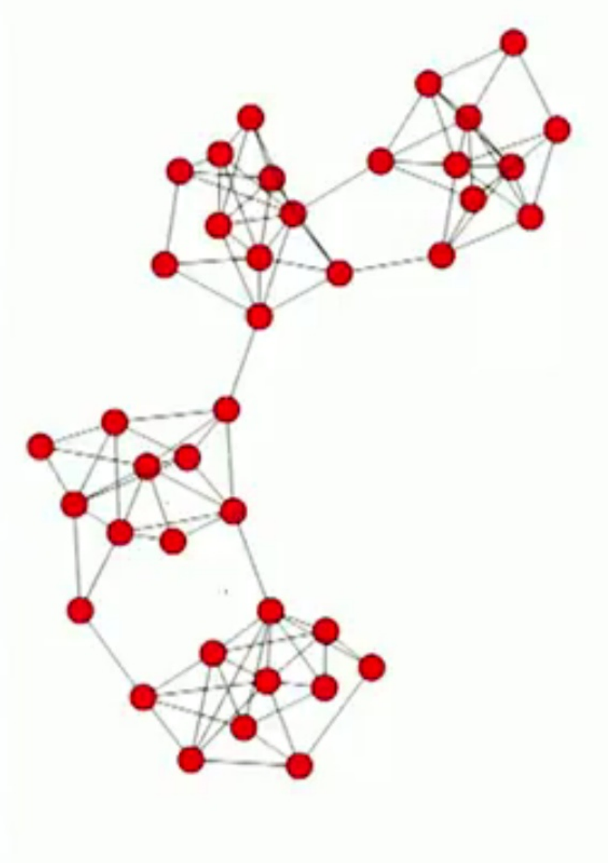
A graph with four communities in R^1

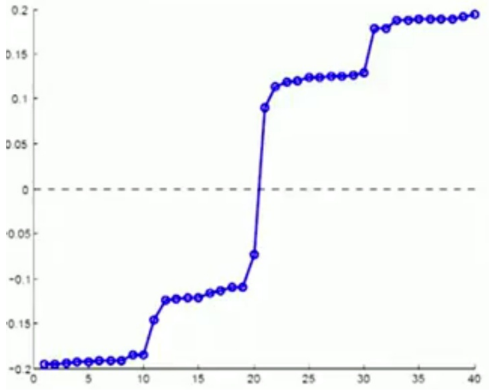




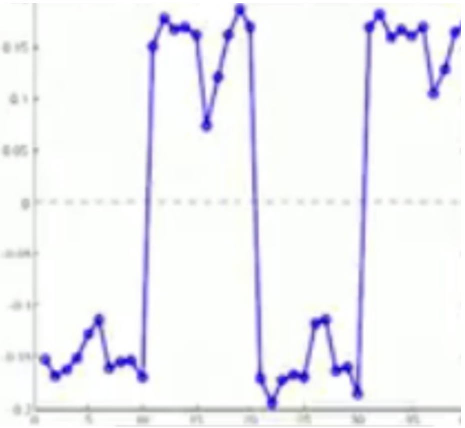
https://www.youtube.com/watch?v=jpTjj5PmcMM

A graph with four communities in R^2

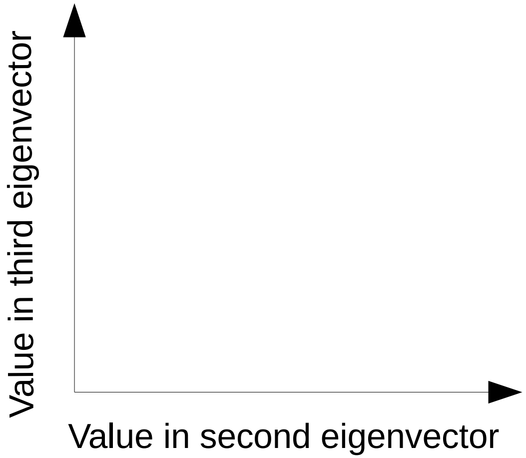




Second eigenvector

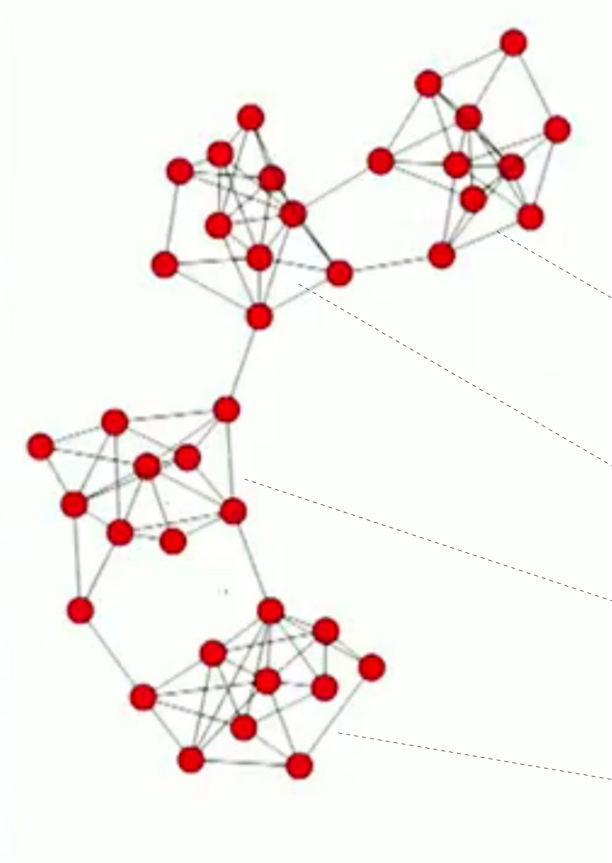


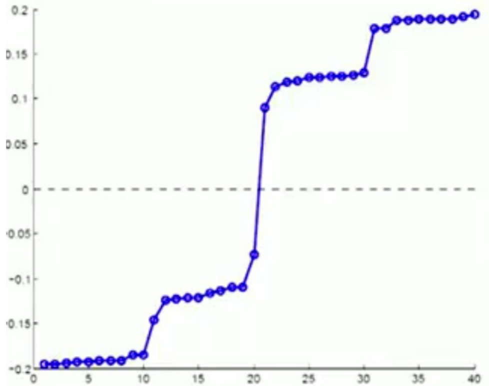
Third eigenvector



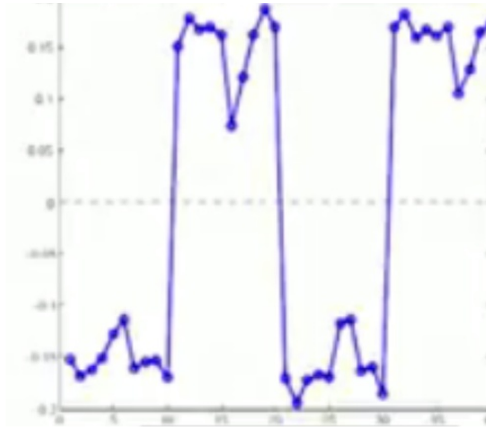
https://www.youtube.com/watch?v=jpTjj5PmcMM

A graph with four communities in R^2 (cont)

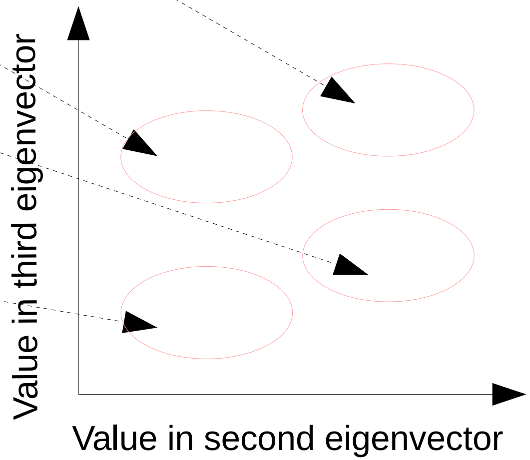




Second eigenvector



Third eigenvector

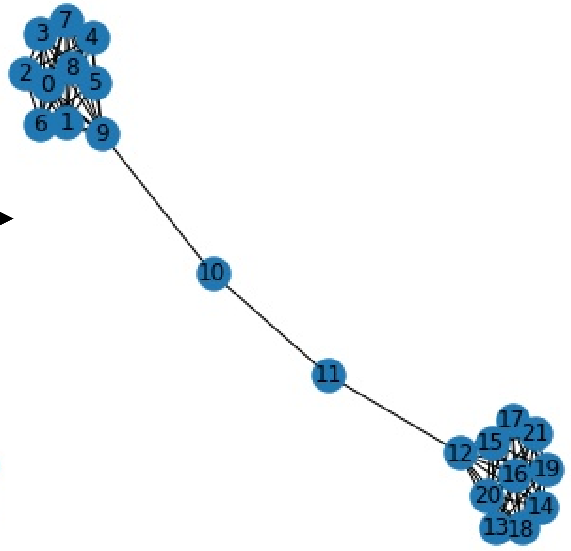


Clustering can be done using Euclidean distance

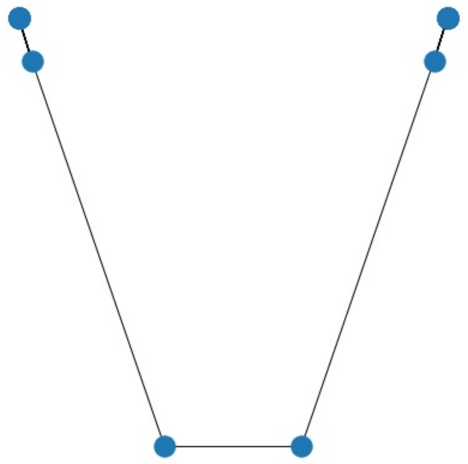
https://www.youtube.com/watch?v=jpTjj5PmcMM

A barbell graph in R^2 (code)

```
B = nx.barbell_graph(10,2)

plt.figure(figsize=(6,6))
nx.draw_networkx(B)
_ = plt.show()
```



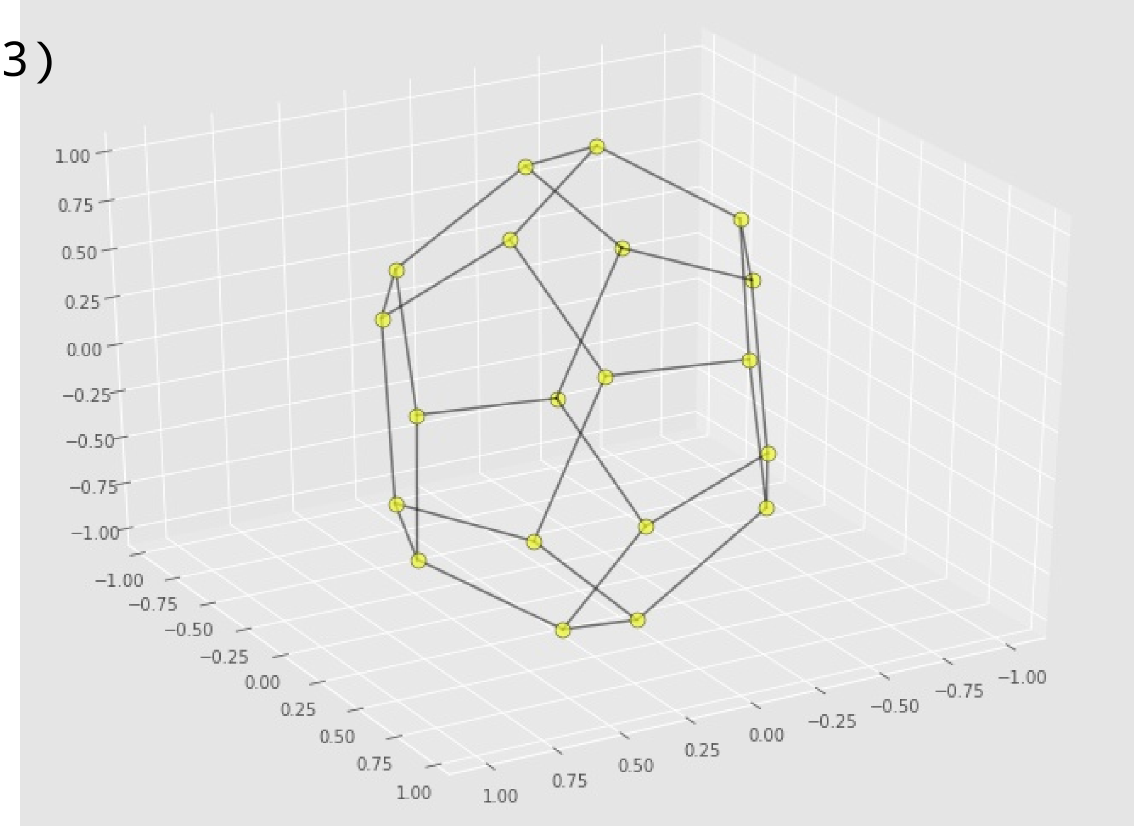

```
plt.figure(figsize=(6,6))
nx.draw_spectral(B)
_ = plt.show()
```



Graph Laplacian

Dodecahedral graph in 3D

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

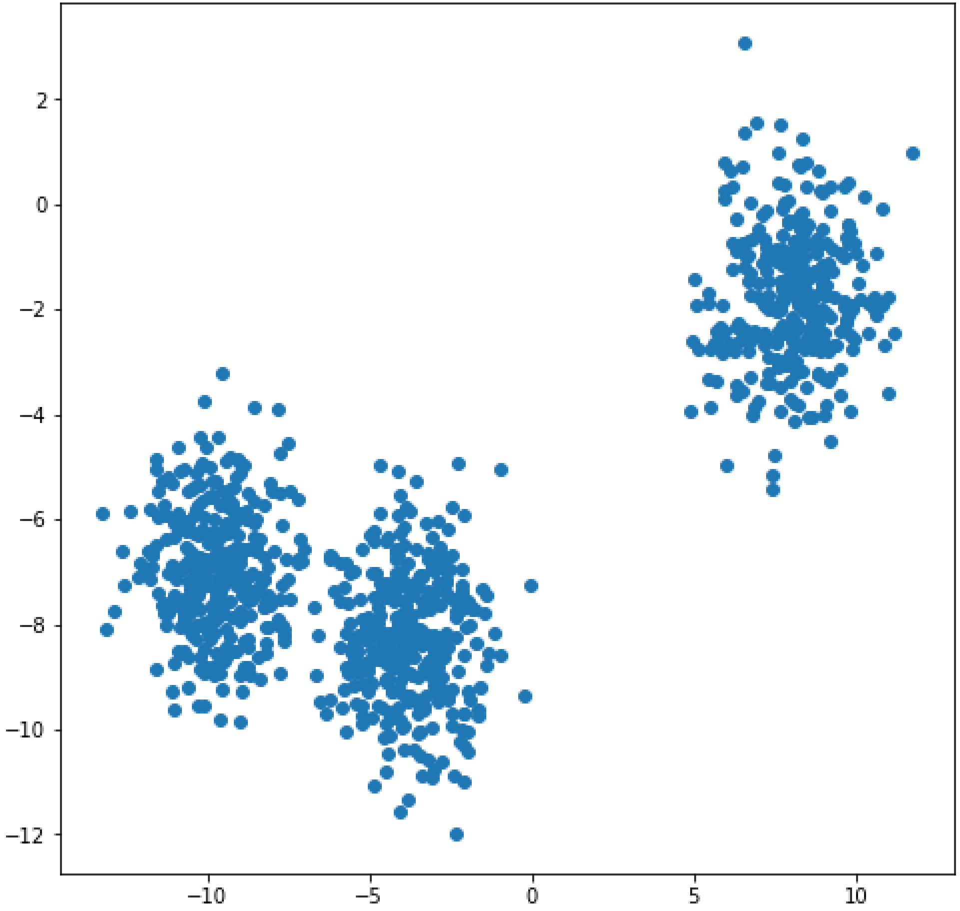


https://www.idtools.com.au/3d-network-graphs-python-mplot3d-toolkit/

Application: spectral clustering

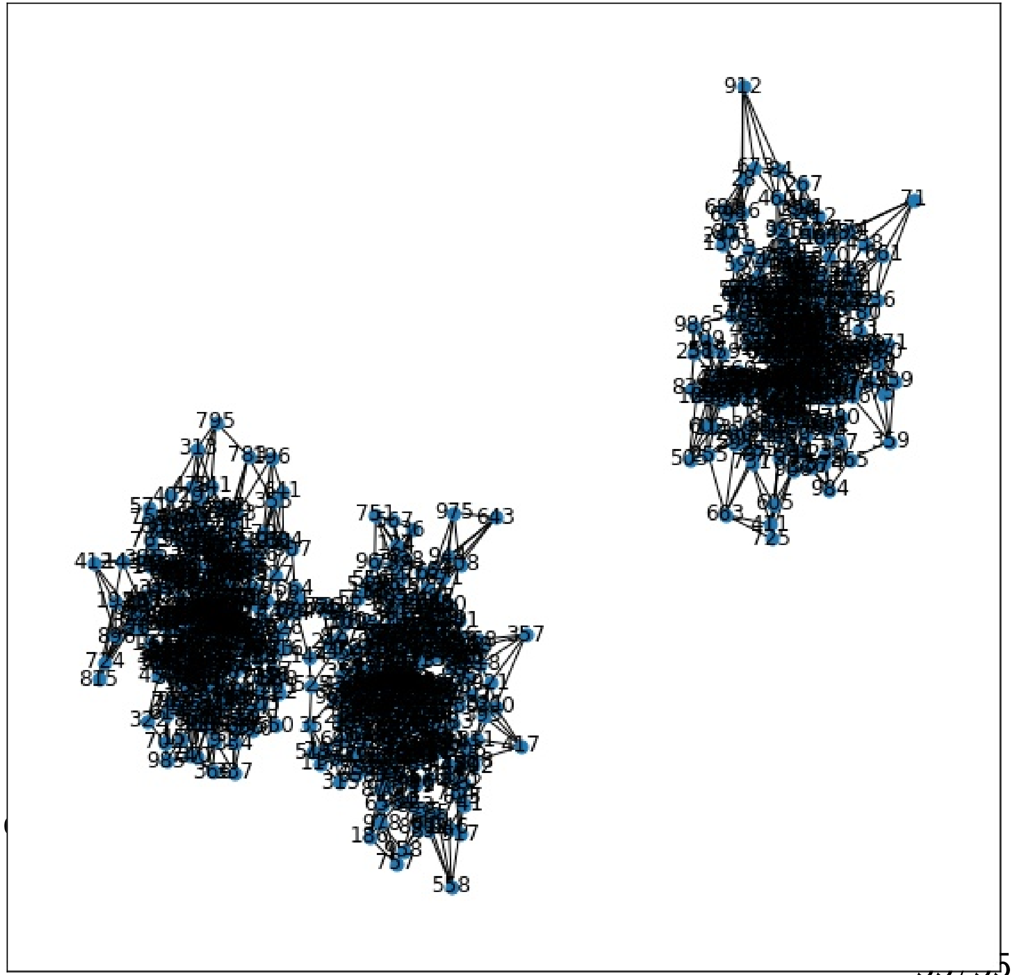
Generating data

```
from sklearn.datasets import
    make_blobs

N = 1000

x, _ = make_blobs(
    n_samples=N,
    centers=3,
    cluster_std=1.2)


plt.figure(figsize=(8,8))

plt.scatter(x[:,0], x[:,1])

plt.show()
```



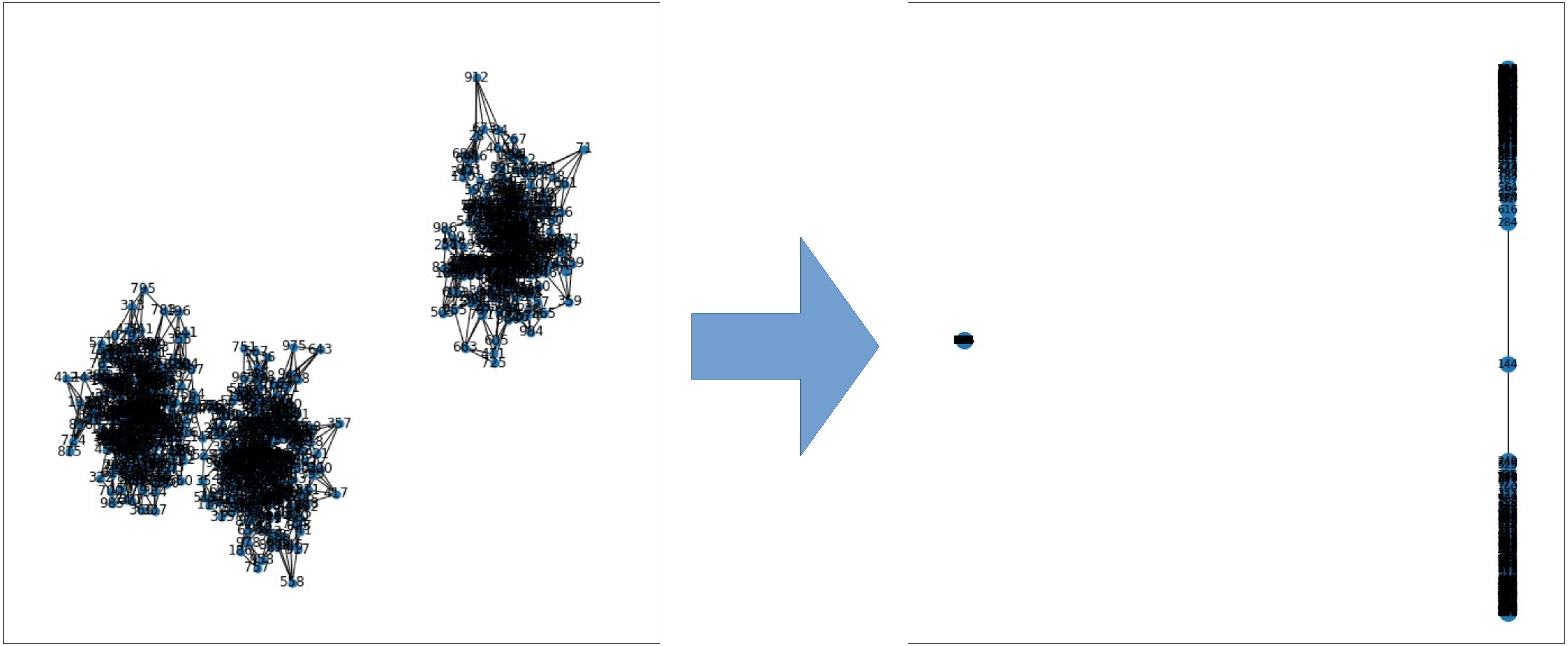
Connect nodes to k=5 nearest neighbors

```
from sklearn.neighbors
   import NearestNeighbors

nbrs = NearestNeighbors(
    n_neighbors=6,         # includes self
    algorithm='ball_tree')
    .fit(x)

distances, neighbors =
    nbrs.kneighbors(x)

G = nx.Graph()

for neighbor_list in neighbors:

    source_node = neighbor_list[0]

    for target_index in range(1,
        len(neighbor_list)):

        target_node = neighbor_list[target_inde

        G.add_edge(source_node, target_node)
```



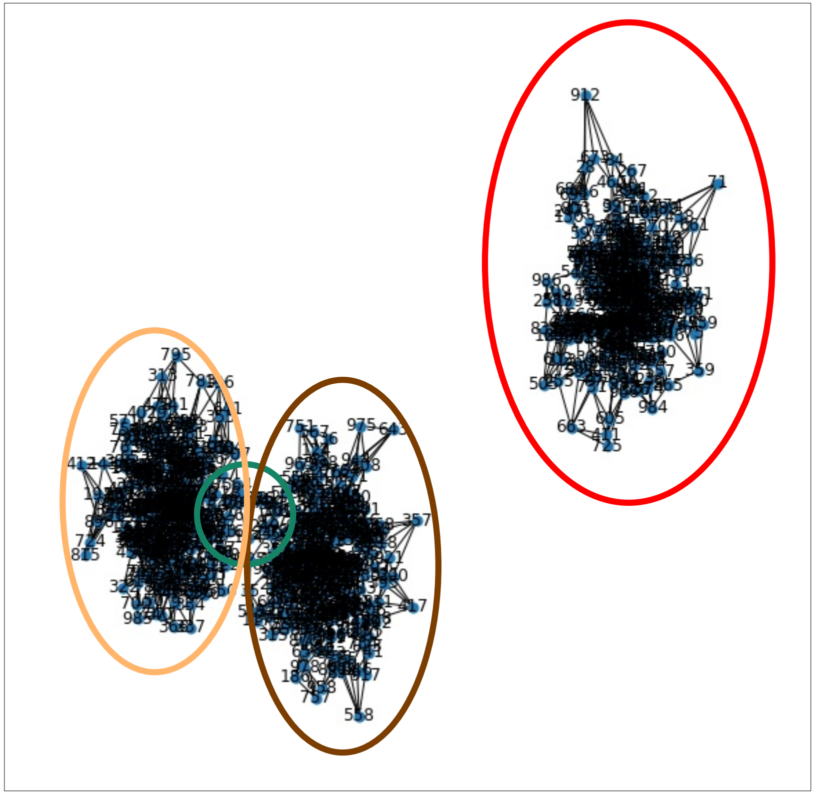
Perform spectral embedding

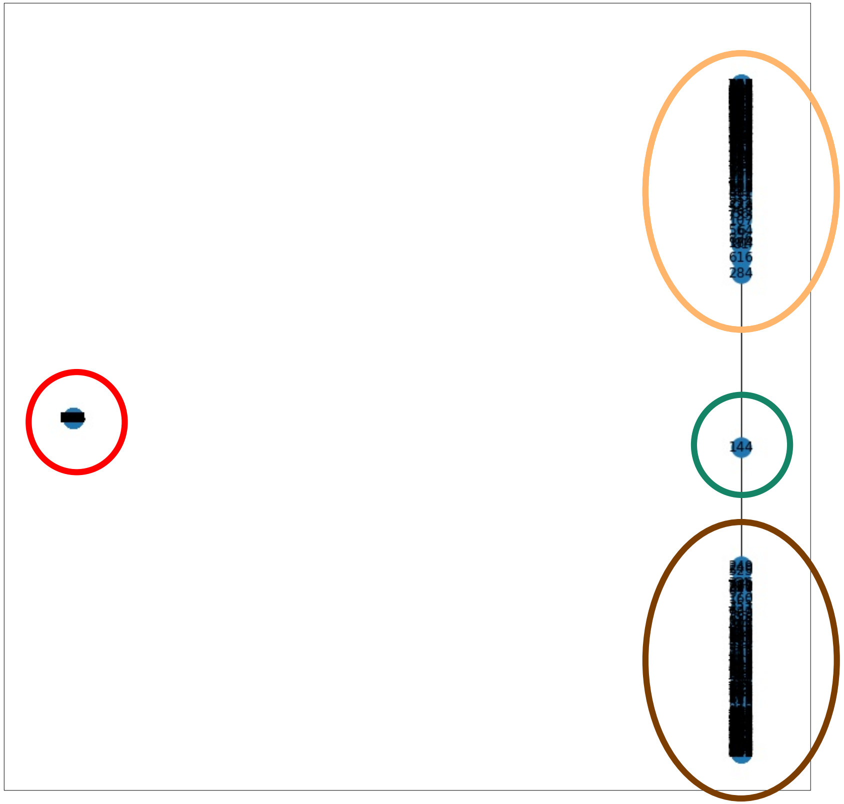
```
nx.draw_spectral(G, with_labels=True)
```



Perform spectral embedding

```
nx.draw_spectral(G, with_labels=True)
```





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