

# Spectral Graph Embedding

## Social Networks Analysis and Graph Algorithms

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



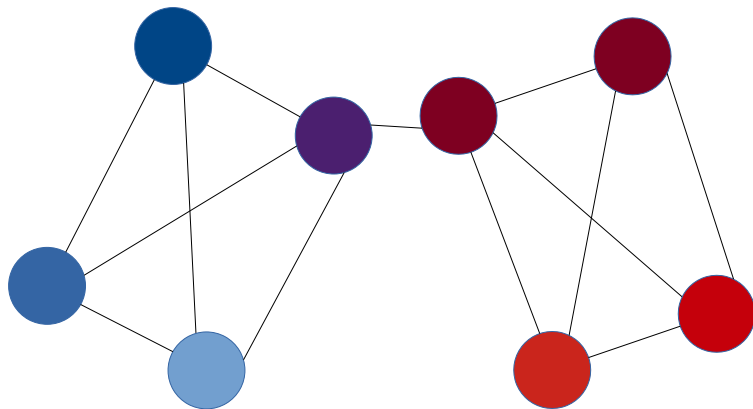
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*Barcelona*

# 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

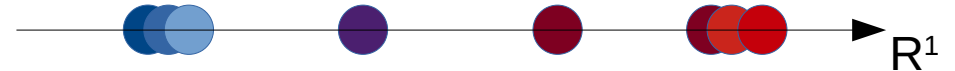
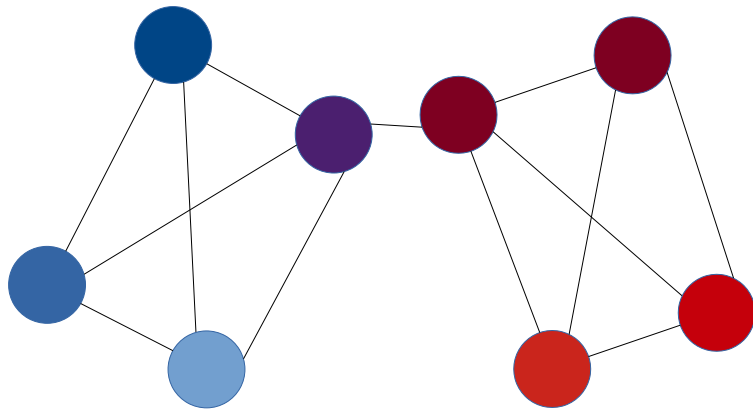
# Graphs are nice, but ...

- 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  $\mathbb{R}^k$



# Graphs are nice, but ...

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**Distances should be somehow preserved**

# What is a graph embedding?

- A graph **embedding** (or graph **projection**) 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

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

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

Draw this graph on paper, upload a photo



What constitutes a good drawing?



Padlet: <https://upfbarcelona.padlet.org/chato/3hwnctvqb7p1z6xx>

# 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 projections

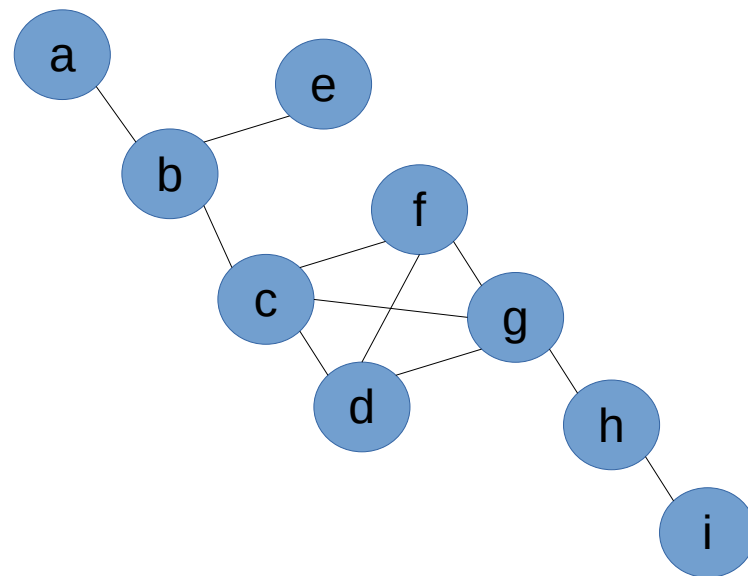


# Random graph projection (2D)

- 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  $\mathbb{R}^2$  plane



Padlet: <https://upfbarcelona.padlet.org/chato/9pd56scbpko5svdj>

# Refresher about eigenvectors/eigenvalues

# Eigenvectors and eigenvalues

- In general  $Av = \lambda v$  means  $A$  has an eigenvector  $v$  of eigenvalue  $\lambda$
- In **symmetric** matrices, **eigenvectors are orthogonal**

Suppose  $\lambda_1 \neq \lambda_2$

$$\lambda_1 v_1^T v_2 = v_1^T A v_2 = v_1^T \lambda_2 v_2 = \lambda_2 v_1^T v_2$$

- This implies  $v_1^T v_2 = 0$

# In symmetric matrices

- The **multiplicity** of an eigenvalue  $\lambda$  is the dimension of the space of eigenvectors of eigenvalue  $\lambda$
- Every  $n \times n$  symmetric matrix has  $n$  eigenvalues counted with multiplicity
- Hence, it has an orthonormal basis of eigenvectors

# Rayleigh quotient

In symmetric matrices  $M$ , the second eigenvalue is

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

# 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?

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



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

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

Can you write  $y_i$  using  $E$  ?

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

# 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  $i^{\text{th}}$  coordinate contains the sum of the  $x_j$  who are in-neighbors of  $i$


# 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?


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

# An eigenvector of a d-regular graph

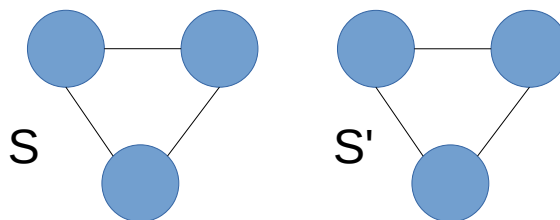
- Suppose graph is d-regular, i.e. all nodes have degree d:

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

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

# Disconnected graphs

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

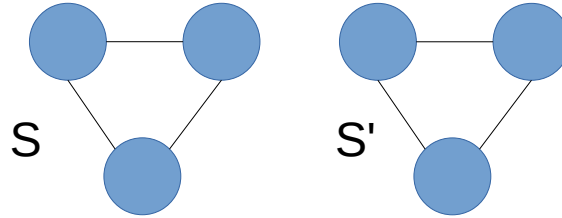


- Then its adjacency matrix has **block structure**:

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

# Disconnected graphs

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

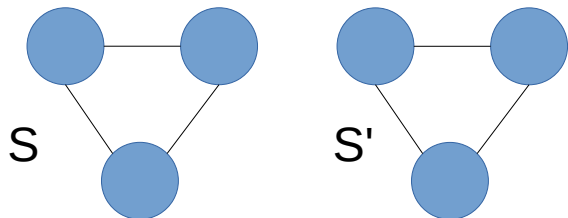


$$\text{Let } x_i^S = \begin{cases} 1 & \text{if } i \in S \\ 0 & \text{if } i \in S' \end{cases}$$

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

# Disconnected graphs

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



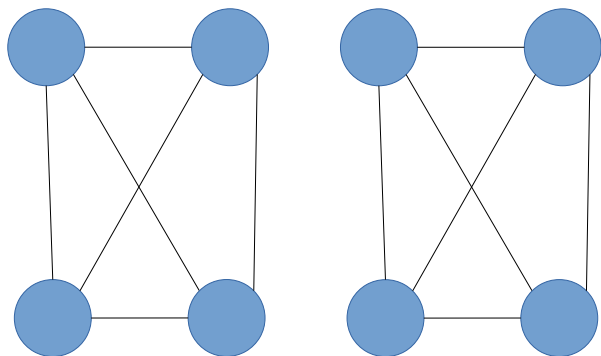
$$Ax^S = dx^S$$

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

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

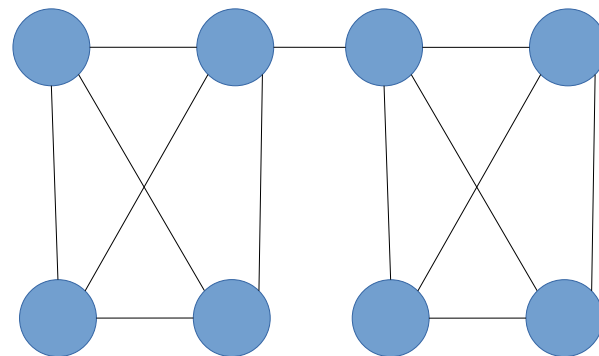
# In general

Disconnected graph



$$\lambda_1 = \lambda_2$$

*Almost* disconnected graph



$$\lambda_1 \approx \lambda_2$$

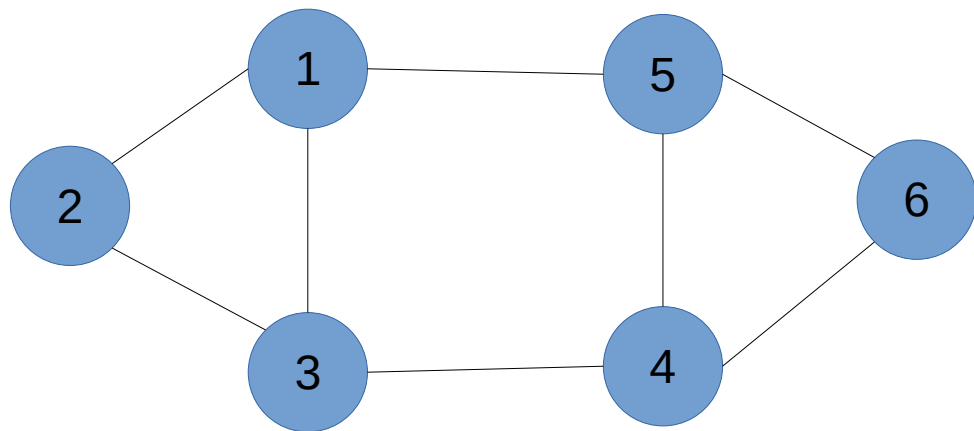
Small “**eigengap**”



# Graph Laplacian

# Adjacency matrix

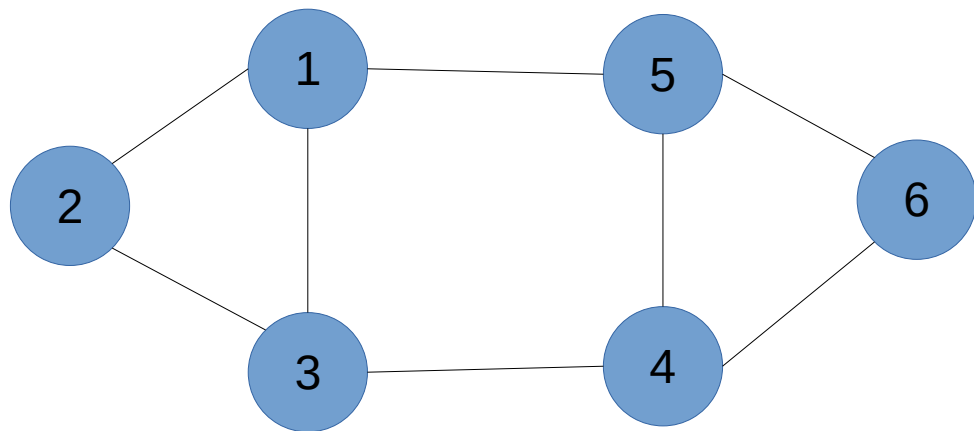
$$A_{ij} = \begin{cases} 1 & \text{if } (i, j) \in E \\ 0 & \text{otherwise} \end{cases}$$



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

# Degree matrix

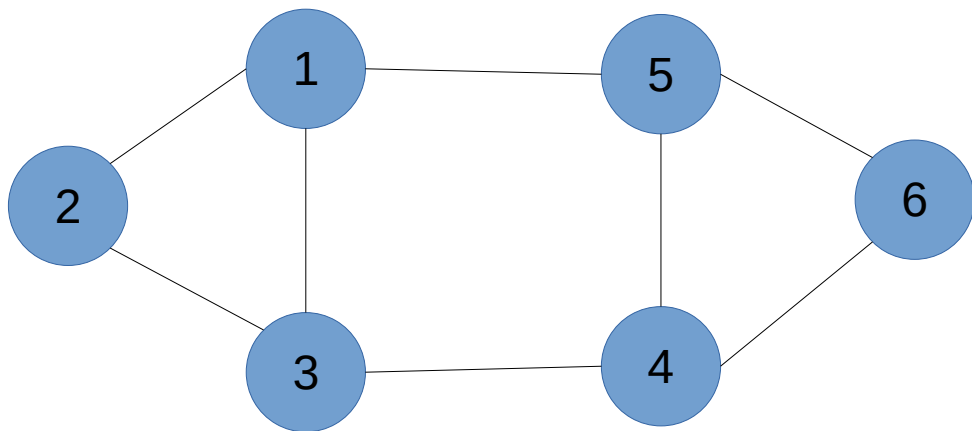
$$D_{ij} = \begin{cases} k_i & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$



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

# Laplacian matrix

$$L = D - A$$



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

Given  $A$  is symmetric,  $L$  is symmetric.

They only differ in the diagonal.

# Laplacian matrix $L = D - A$

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

# The constant vector is an eigenvector of L

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

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

Does it need to be this specific graph? Why?

Does it need to be the vector  $[1, 1, \dots, 1]^T$ ? Why?

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

$$L = D - A$$

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

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

# One of the eigenvalues of $L$ is 0

- If  $x$  is such that  $x_i = x_j$  for all  $i, j$ :

$$x^T Lx = \sum_{(i,j) \in E} (x_i - x_j)^2 = 0 \Rightarrow Lx = 0$$

- This means 0 is an eigenvalue of  $L$

In the Laplacian of a connected graph,  
the eigenvector of  $\lambda=0$  must be the constant vector

- Suppose  $Lx = 0$
- Then  $x^T Lx = \sum_{(i,j) \in E} (x_i - x_j)^2 = 0$

How do we get from this that if the graph is connected,  
 $x_i = x_j$  for any  $i, j$  ?

In the Laplacian of a connected graph,  
the eigenvector of  $\lambda=0$  must be the constant vector

- Suppose  $Lx = 0$
- Then  $x^T Lx = \sum_{(i,j) \in E} (x_i - x_j)^2 = 0$
- Hence, for every pair of nodes  $(i,j)$  connected by an edge,  
 $x_i = x_j$
- Hence for all nodes  $x_i = x_j$

# Eigenvalues of the Laplacian are non-negative

- If  $v$  is an eigenvector of  $L$  of eigenvalue  $\lambda$ :

$$\lambda v^T v = v^T L v = \sum_{(i,j) \in E} (v_i - v_j)^2 \geq 0$$

- This means all eigenvalues are non-negative

# In summary, the Laplacian matrix $L = D - A$

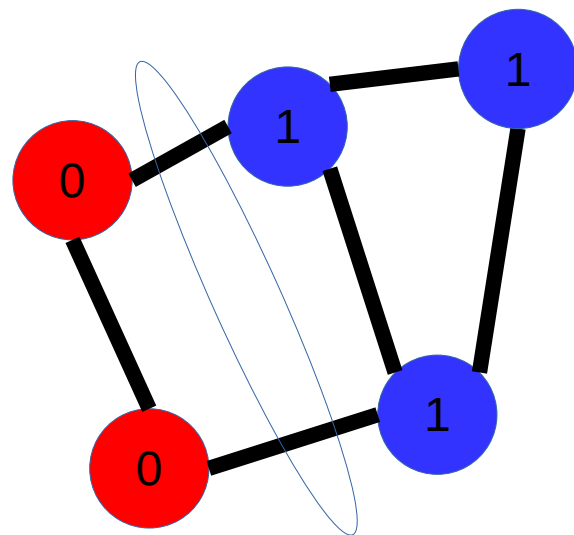
- Is symmetric, eigenvectors are orthogonal
- It has  $N$  eigenvalues that are non-negative
- $0$  is one eigenvalue, with multiplicity equal to the number of connected components of the graph

$$0 = \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_N$$

# The second eigenvector in a connected graph

# $x^T L x$ and graph cuts

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



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

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



# Remember

- For symmetric matrices

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

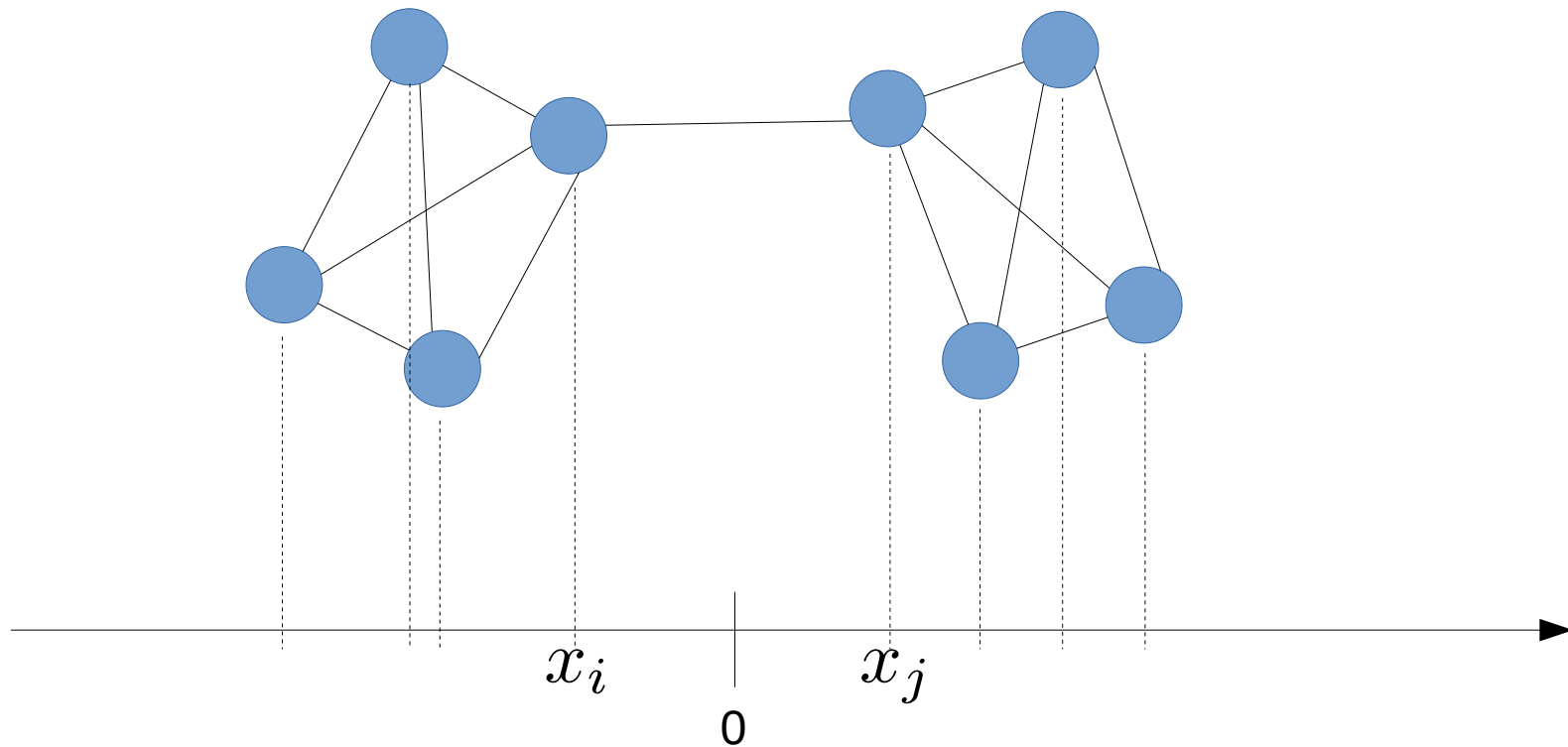
# Second eigenvector

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

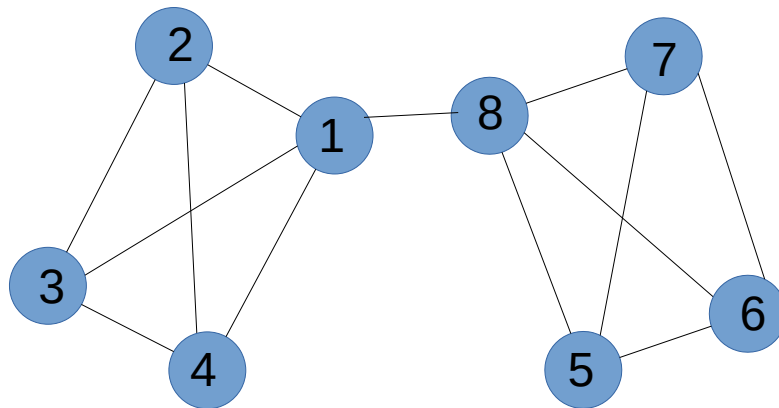
$$\lambda_2 = \min_x \frac{x^T L x}{x^T x} = \min_{x: \sum x_i = 0} \frac{x^T L x}{\sum x_i^2} = \min_{x: \sum x_i = 0} \sum_{(i,j) \in E} (x_i - x_j)^2$$

# What does this mean?

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

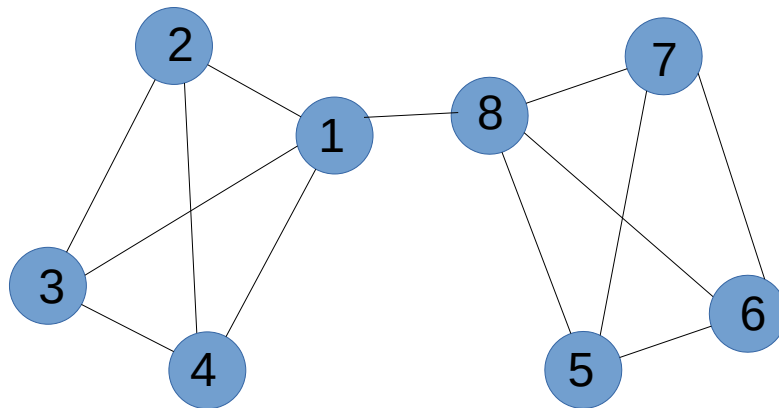


# Example Graph 1



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

# Example Graph 1 (second eigenvalue)



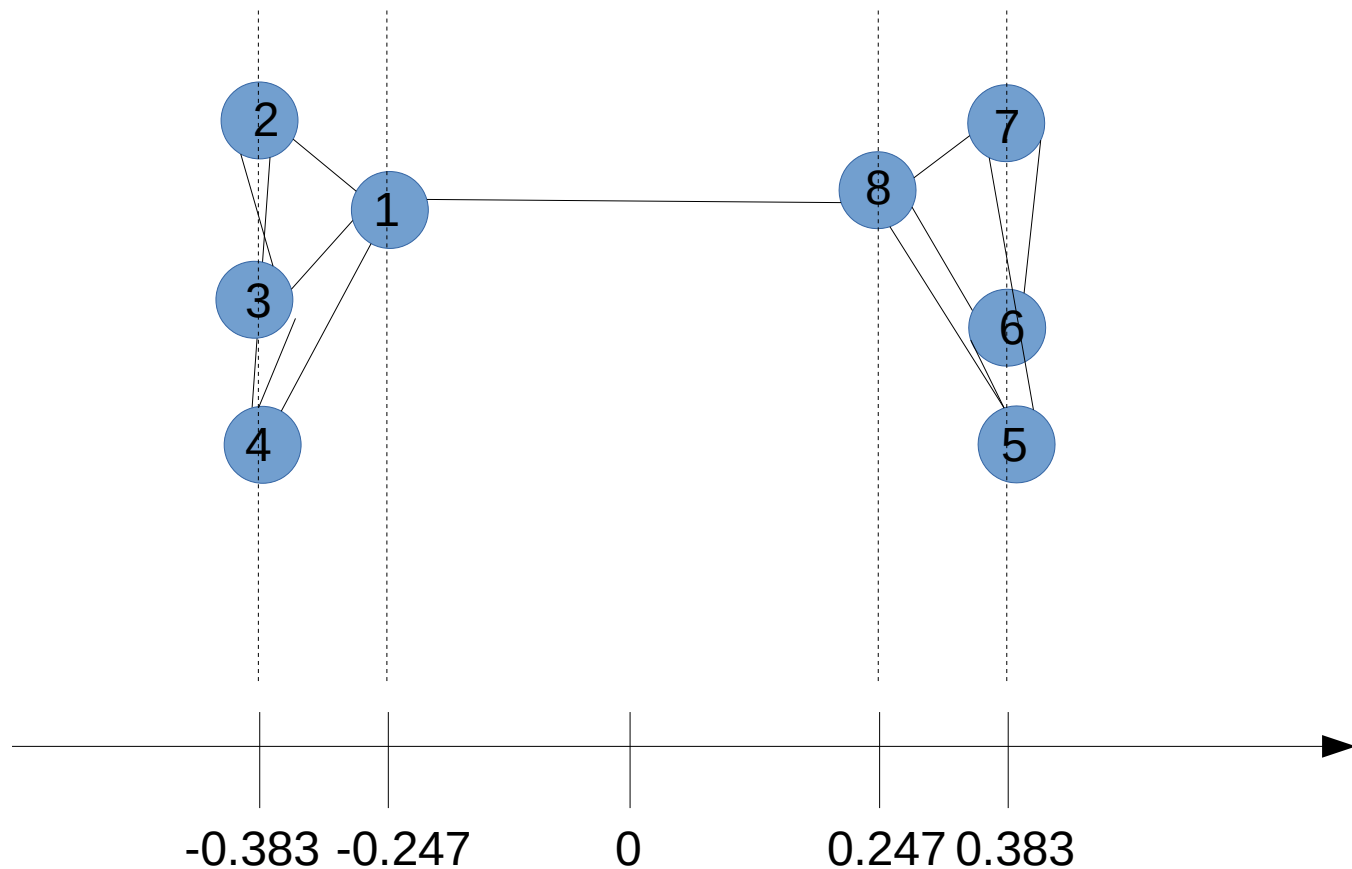
$$\lambda_1 = 0$$

$$\lambda_2 = 0.354$$

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

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

# Example Graph 1, projected in $\mathbb{R}^1$

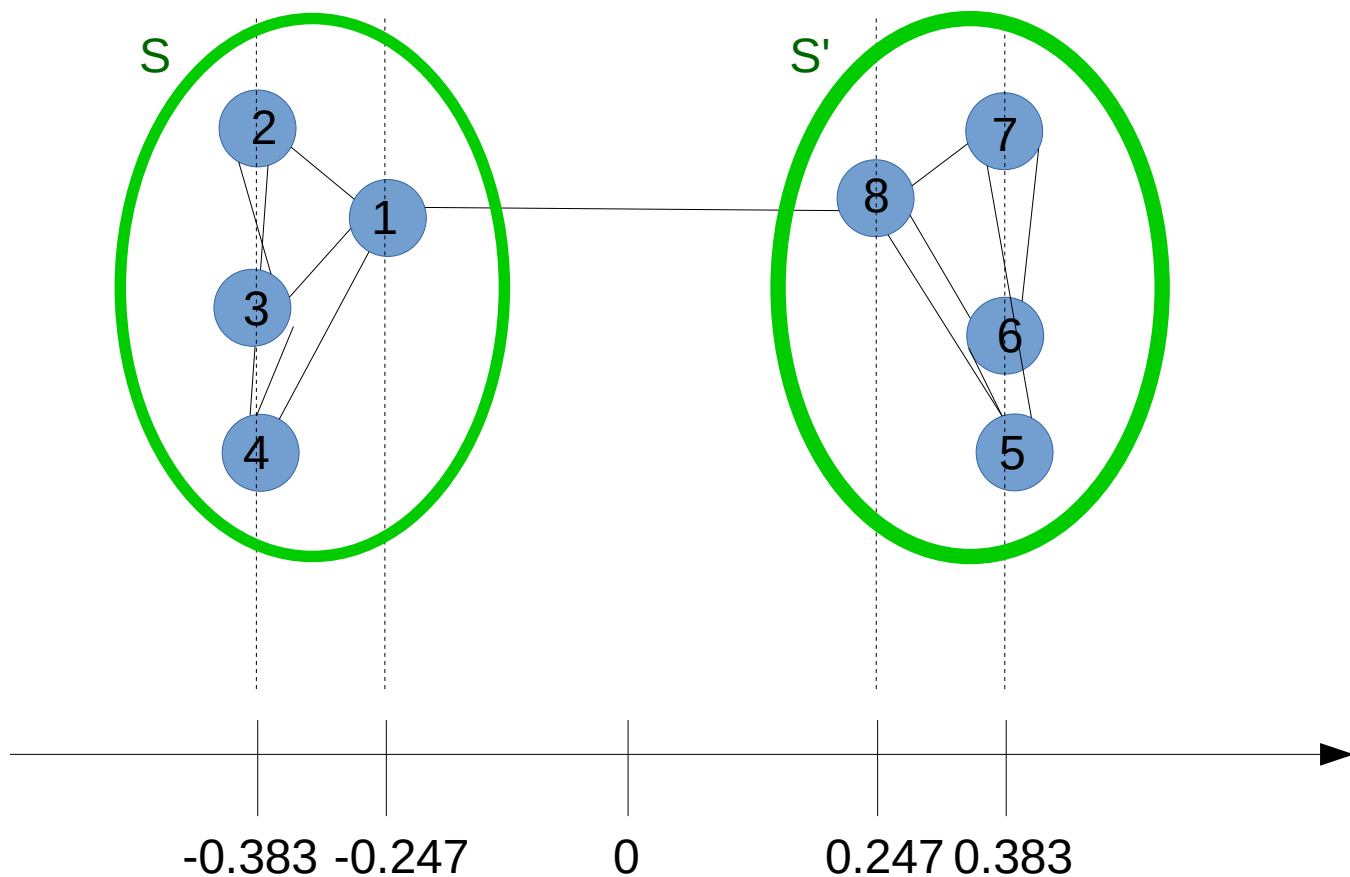


$$\lambda_1 = 0$$

$$\lambda_2 = 0.354$$

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

# Example Graph 1, communities

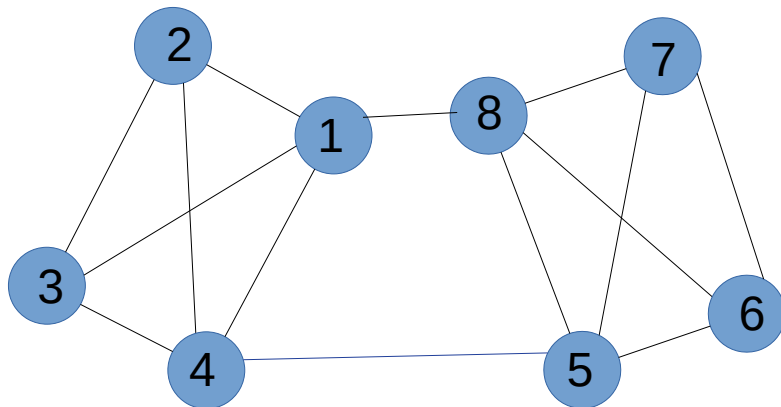


$$\lambda_1 = 0$$

$$\lambda_2 = 0.354$$

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

# Example Graph 2



$$\lambda_1 = 0$$

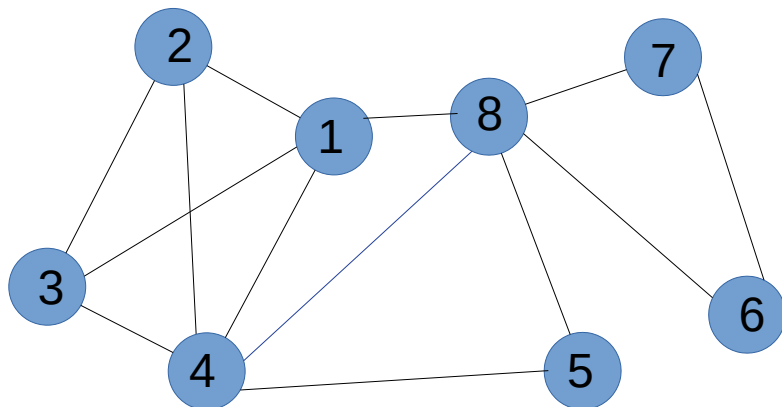
$$\lambda_2 = 0.764$$

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

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



# Example Graph 3



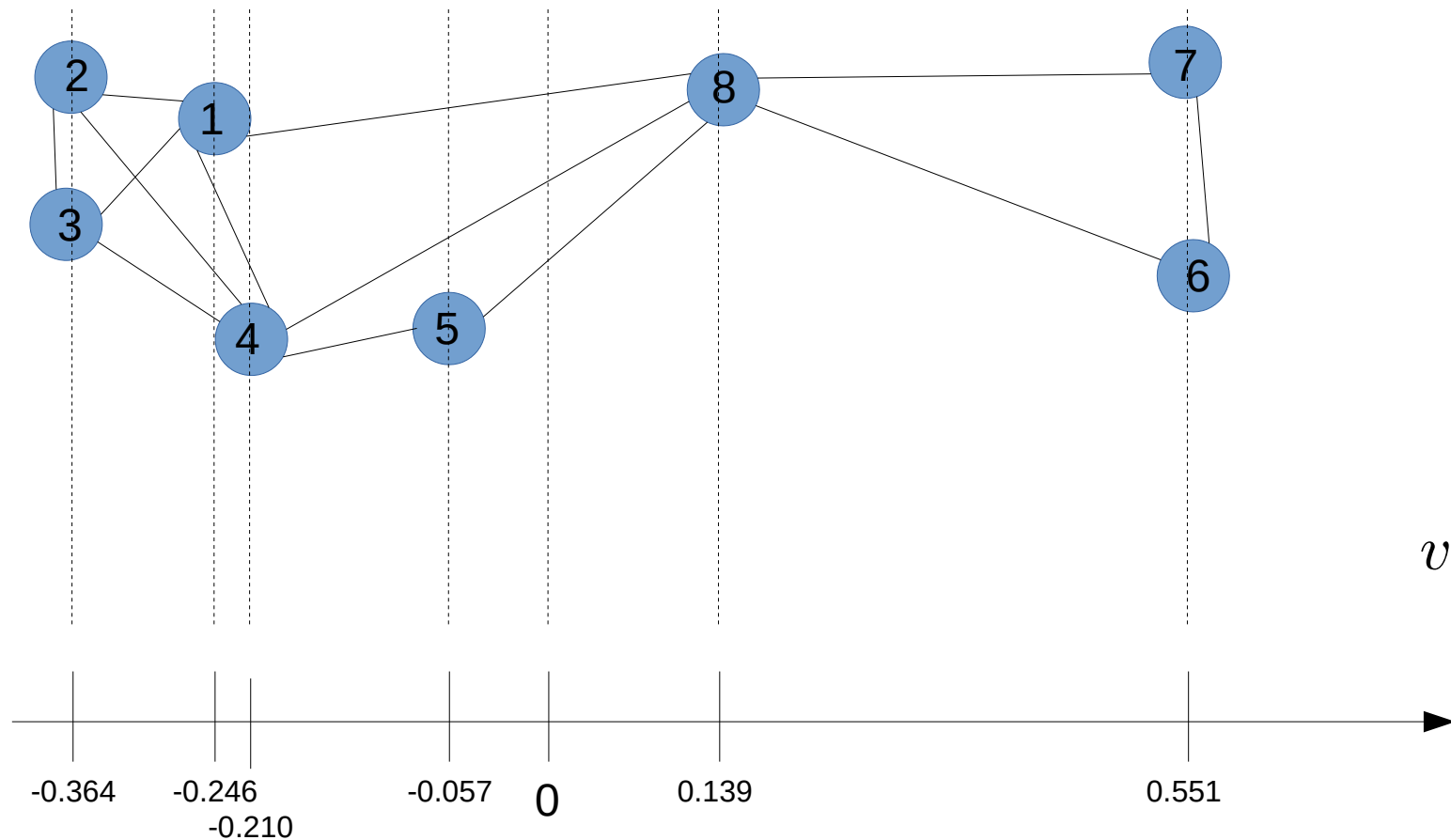
$$\lambda_1 = 0$$

$$\lambda_2 = 0.748$$

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

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

# Example Graph 3, projected (where to cut?)

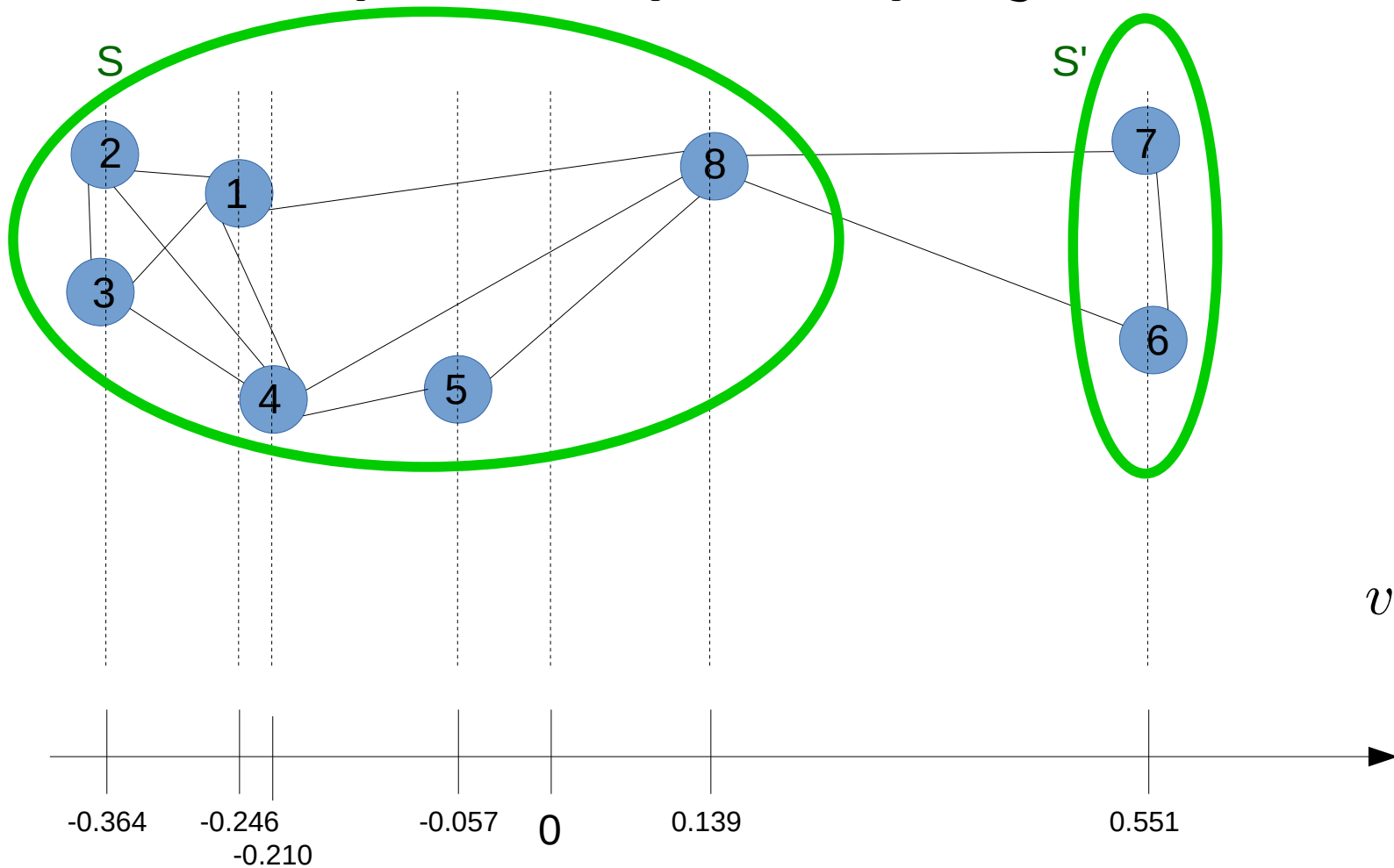


$$\lambda_1 = 0$$

$$\lambda_2 = 0.748$$

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

# Example Graph 3, projected (where to cut?)



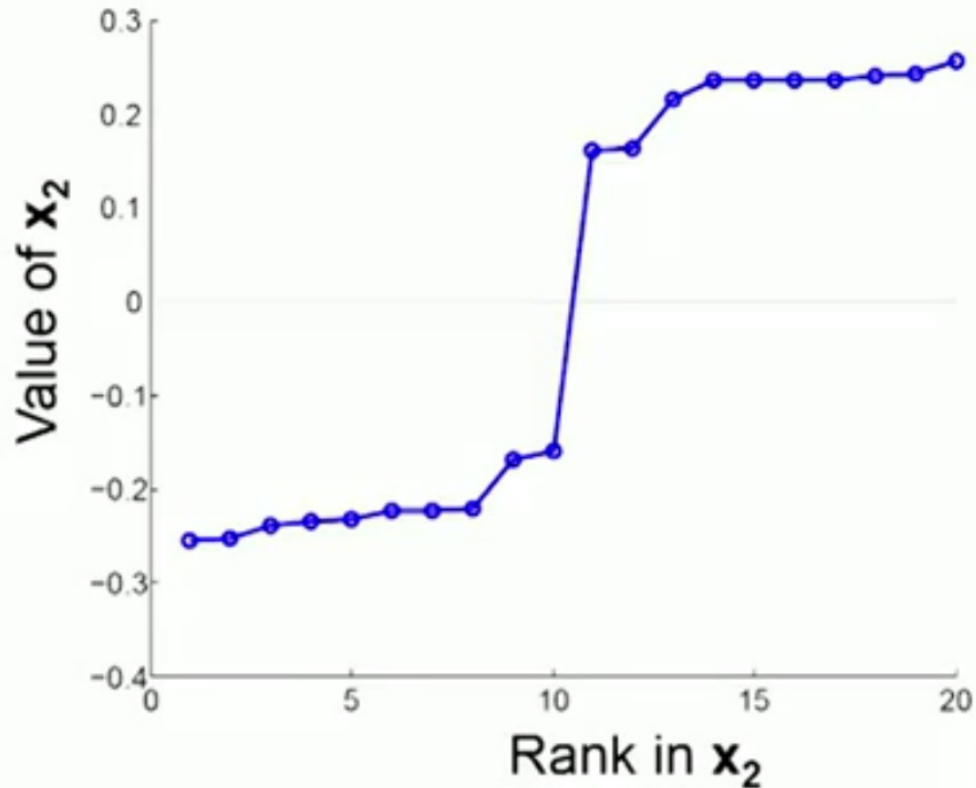
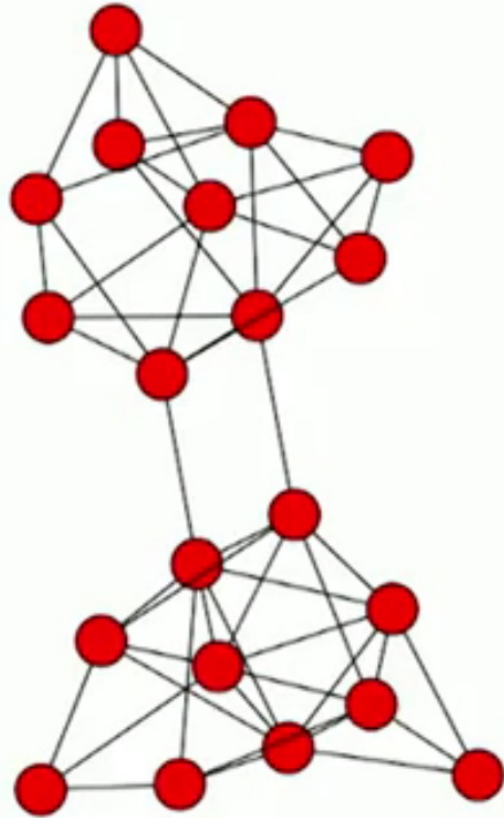
$$\lambda_1 = 0$$

$$\lambda_2 = 0.748$$

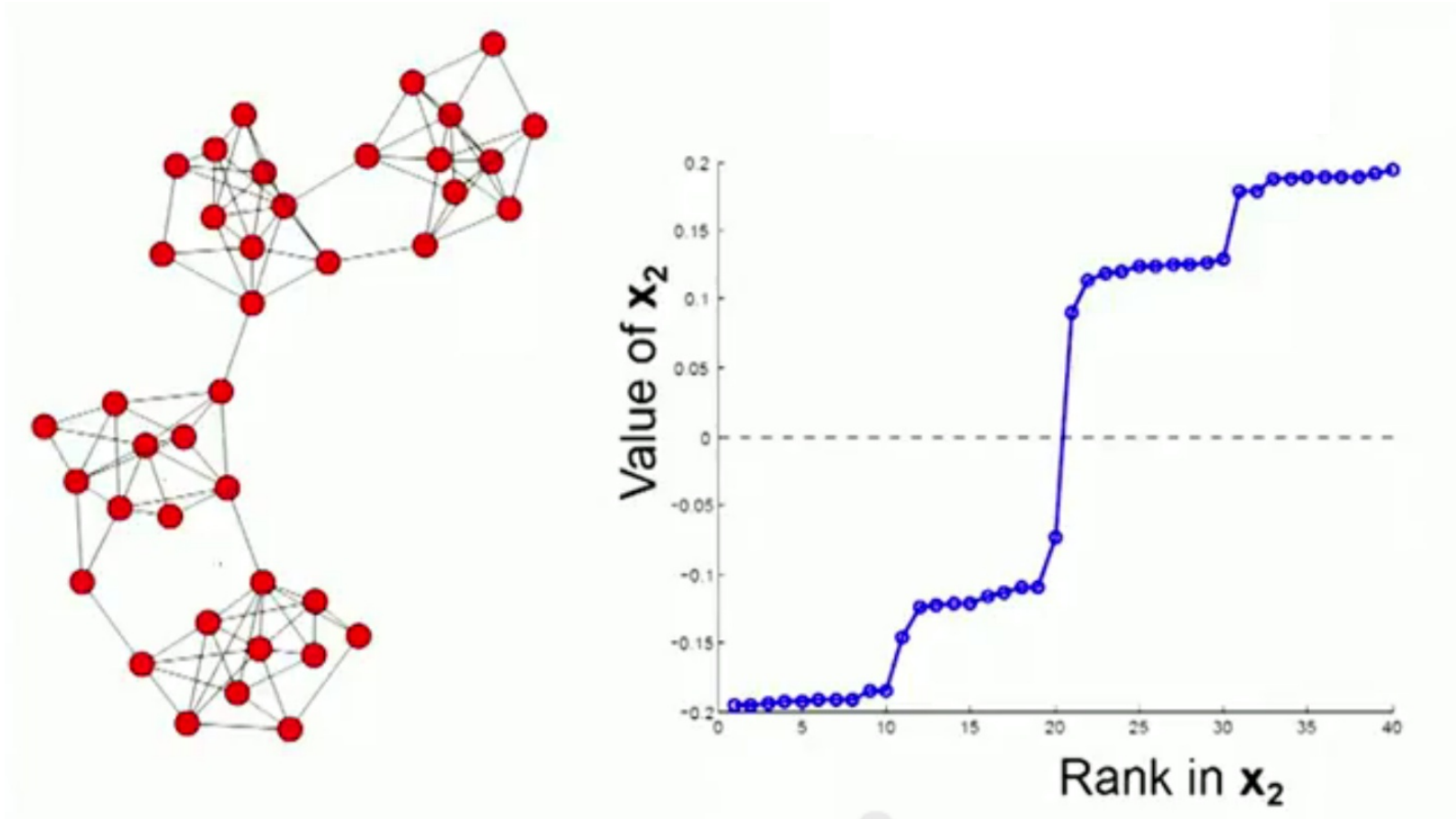
$$v_2 =$$

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

# A graph with two communities in $\mathbb{R}^1$

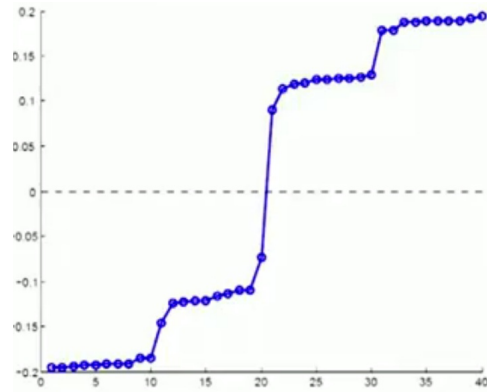
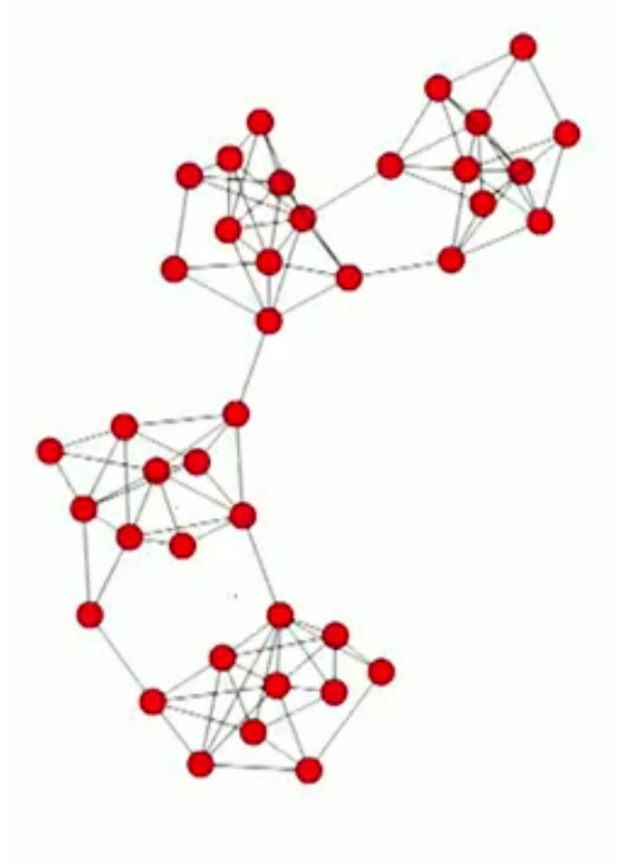


# A graph with four communities in $\mathbb{R}^1$

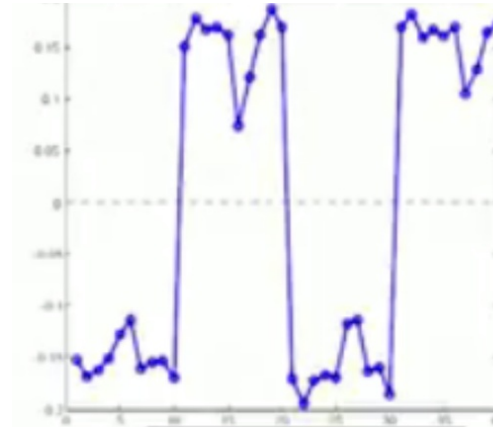


**Application: graph drawing**

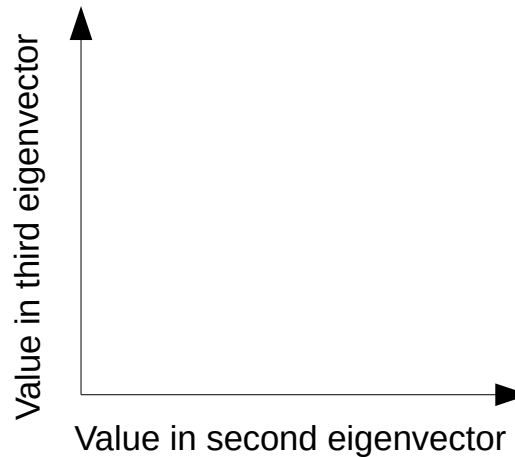
# A graph with four communities in $\mathbb{R}^2$



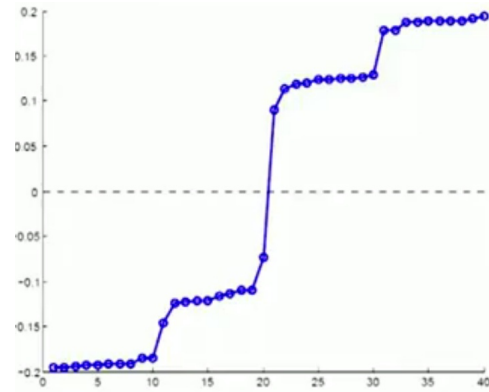
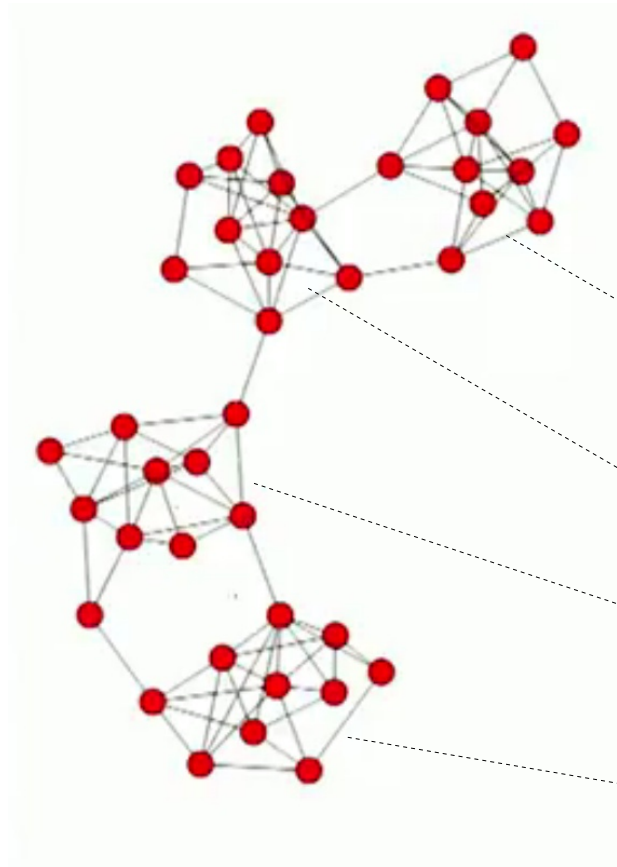
Second eigenvector



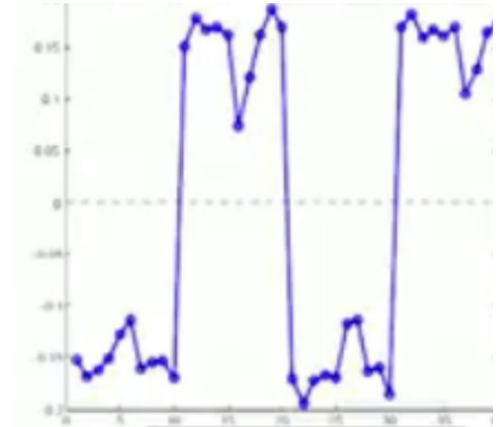
Third eigenvector



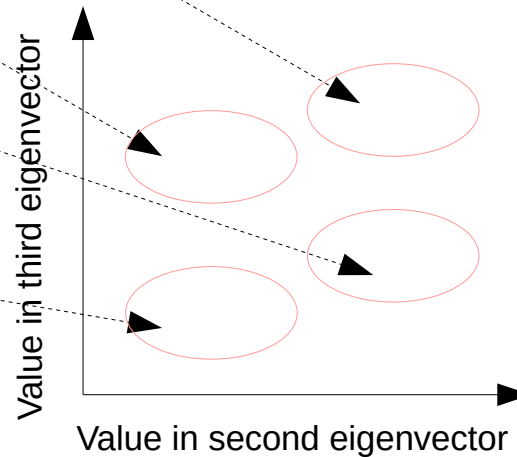
# A graph with four communities in $\mathbb{R}^2$ (cont)



Second eigenvector



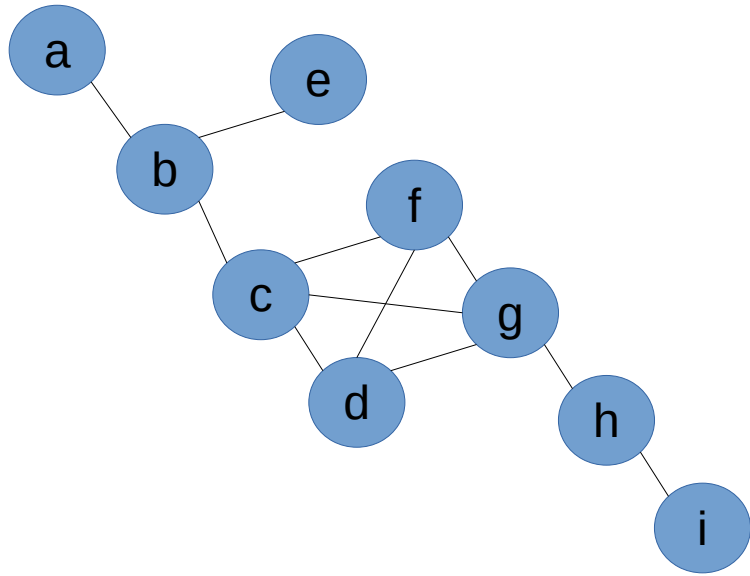
Third eigenvector



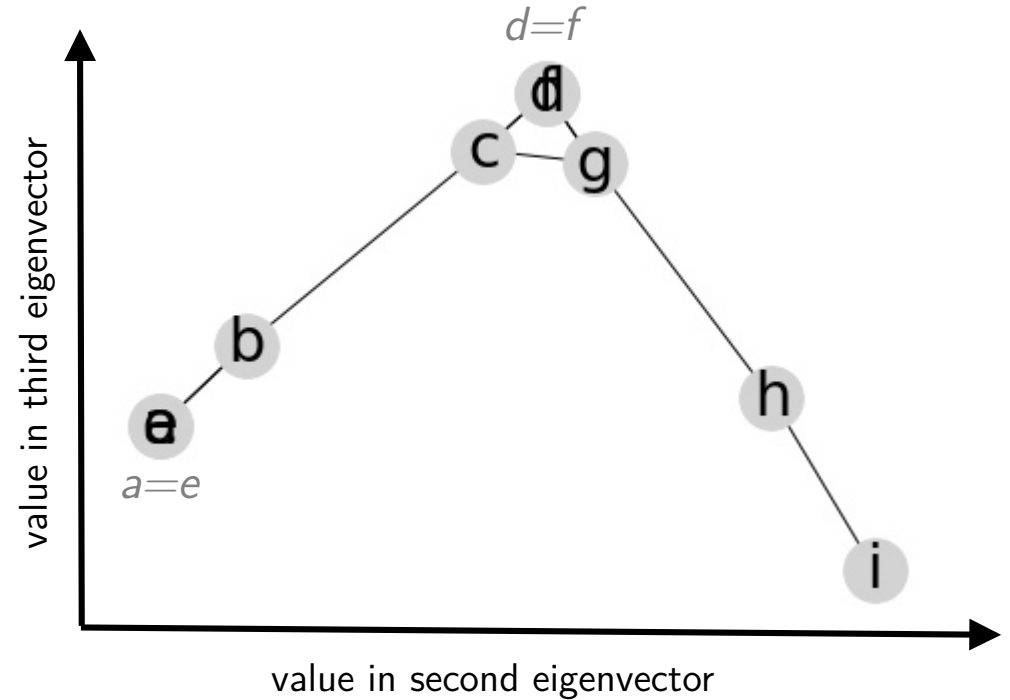
This can be used to draw the graph in  $\mathbb{R}^2$



# The graph from the initial exercise



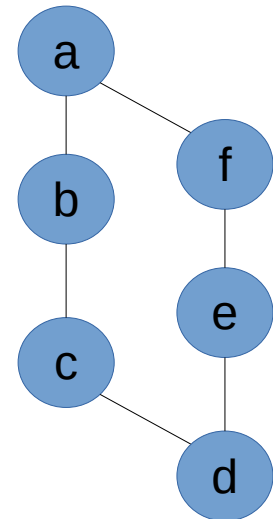
Input nodes and edges



Spectral embedding

# Exercise: spectral projection

- Write the Laplacian
- Get the second and third eigenvector
- Obtain projection



Link to spreadsheet: <https://upfbarcelona.padlet.org/chato/shyq9m6f2g2dh1bw>

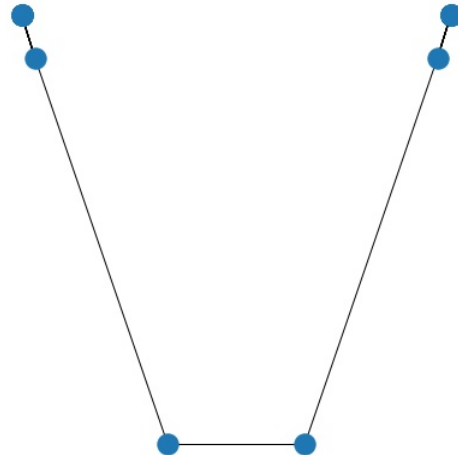
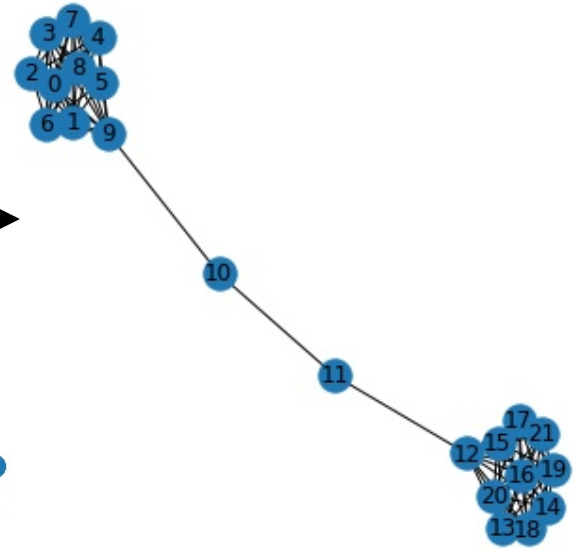


# A barbell graph in $R^2$ (code)

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

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

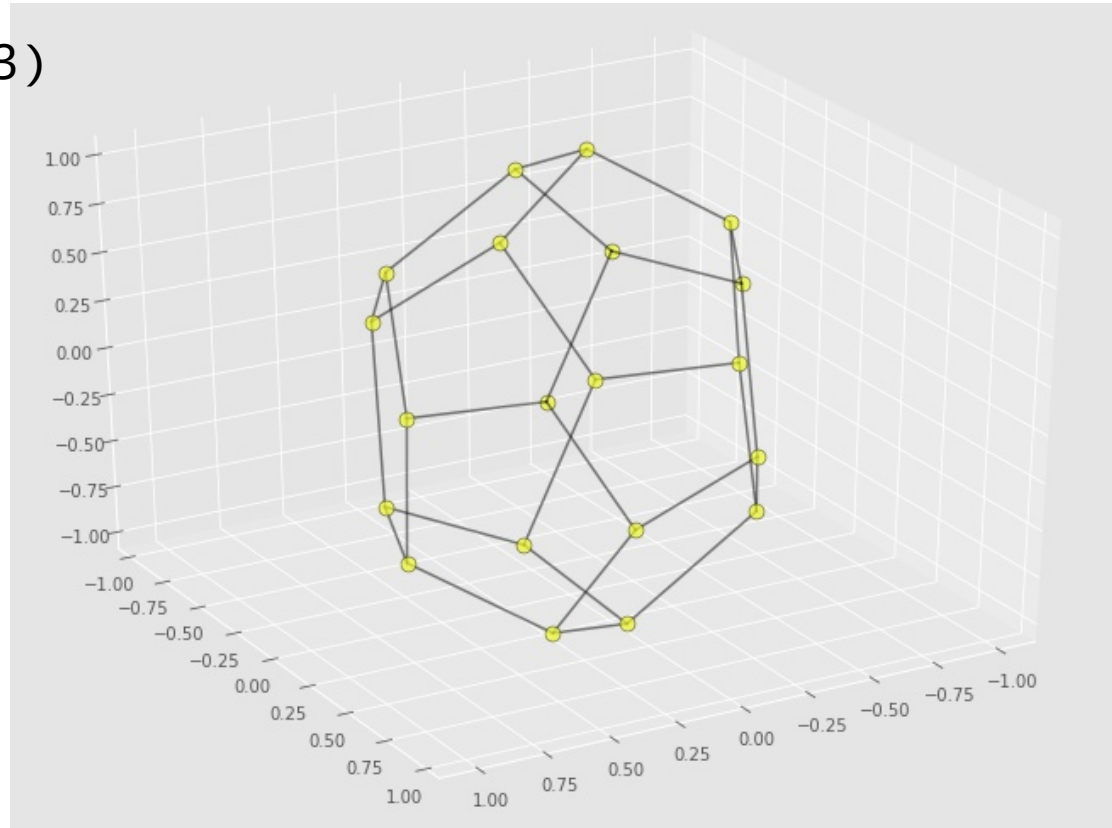
```
plt.figure(figsize=(6,6))  
nx.draw_spectral(B)  
_ = plt.show()
```



Graph Laplacian

# Dodecahedral graph in 3D

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



# Application: spectral clustering

# Generating data

```
from sklearn.datasets import  
    make_blobs
```

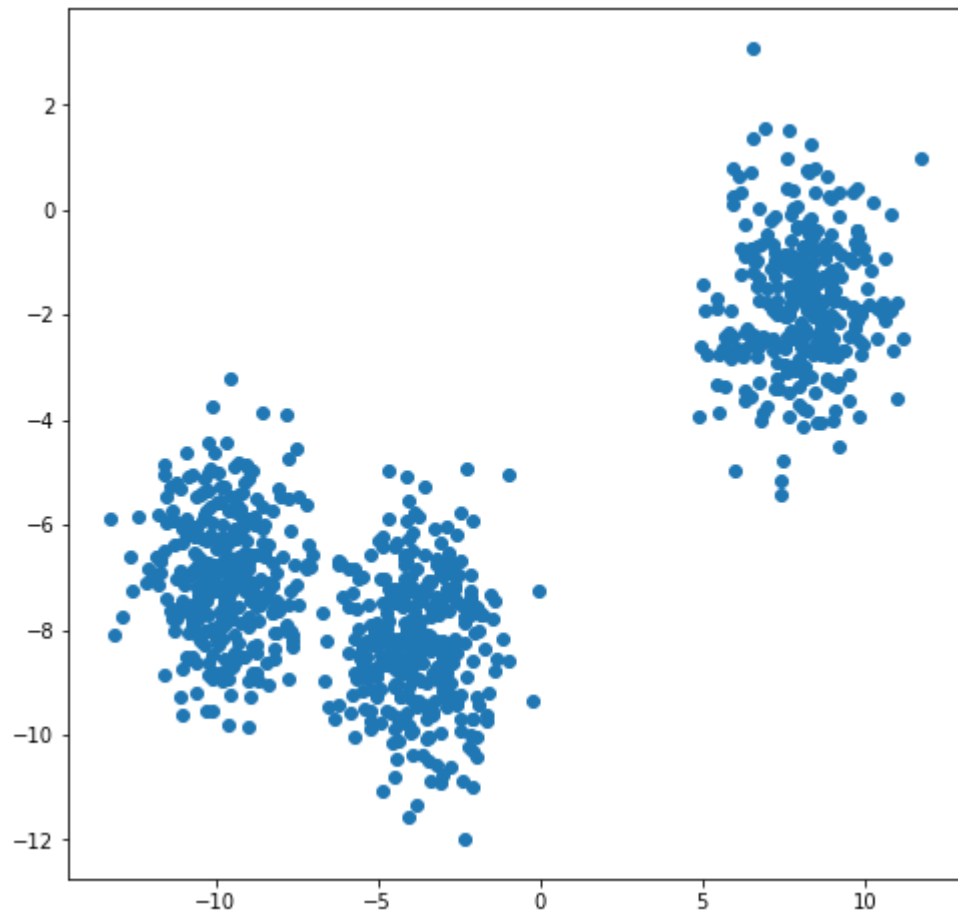
```
N = 1000
```

```
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

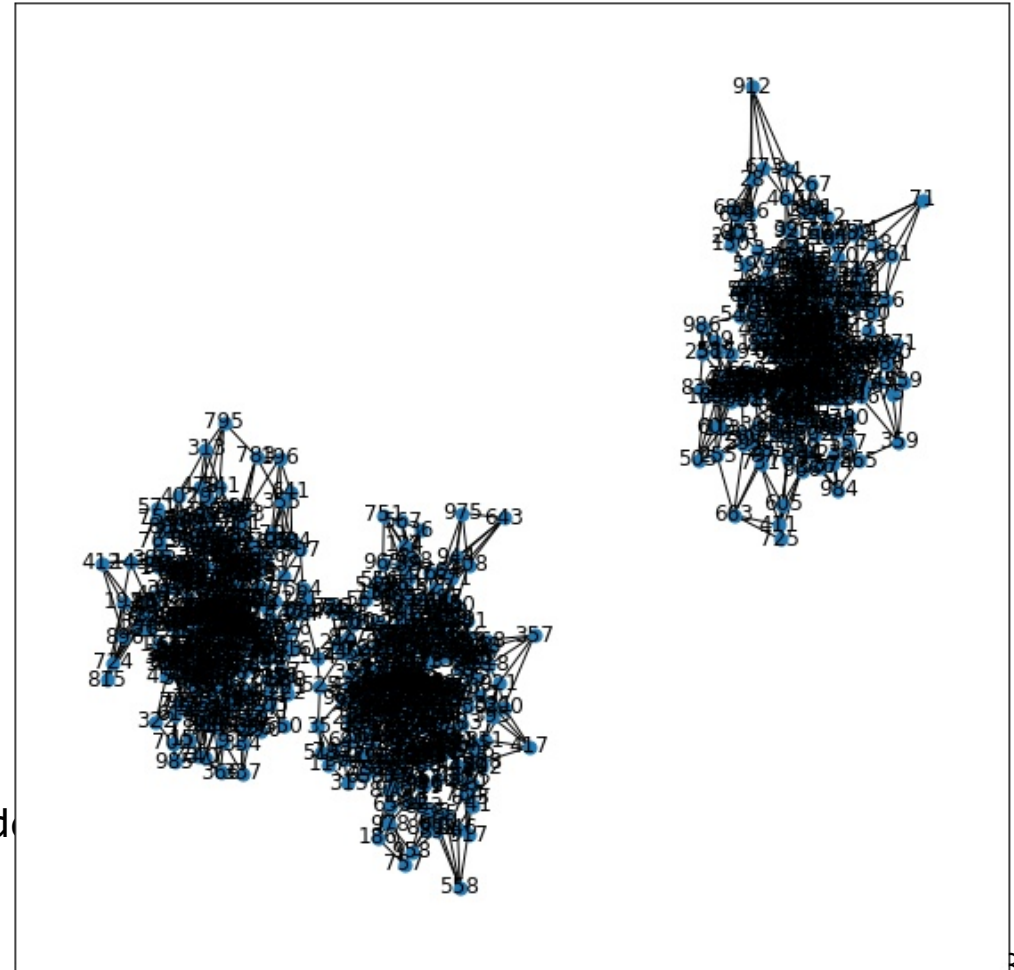
```
from sklearn.neighbors
    import NearestNeighbors

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

distances, neighbors =
    nbrs.kneighbors(x)

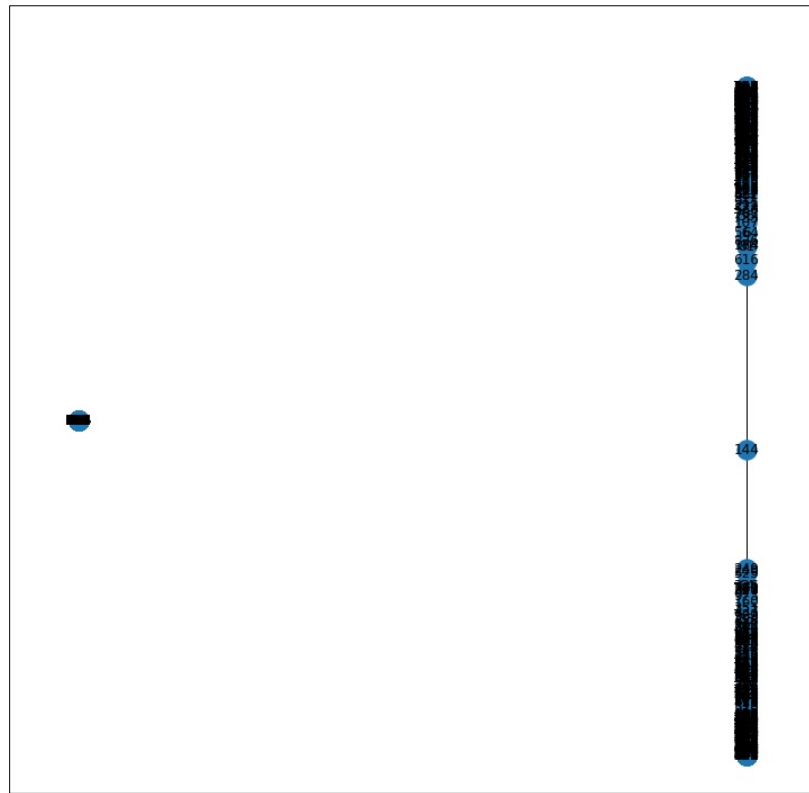
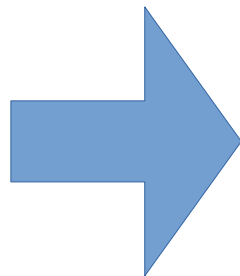
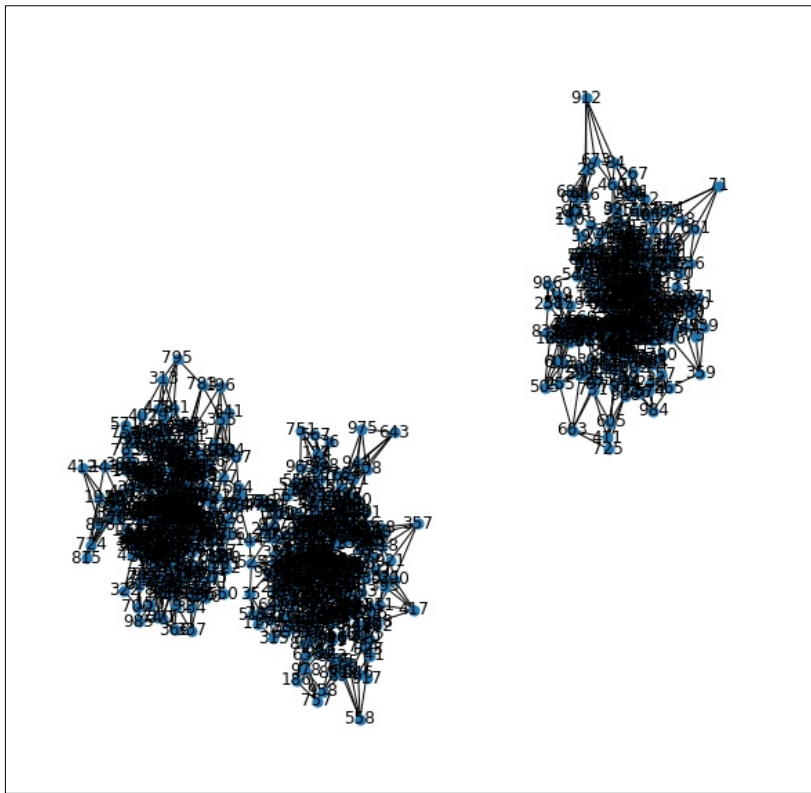
G = nx.Graph()

for neighbor_list in neighbors:
    source_node = neighbor_list[0]
    for target_index in range(1,
        len(neighbor_list)):
        target_node = neighbor_list[target_index]
        G.add_edge(source_node, target_node)
```



# Perform spectral embedding

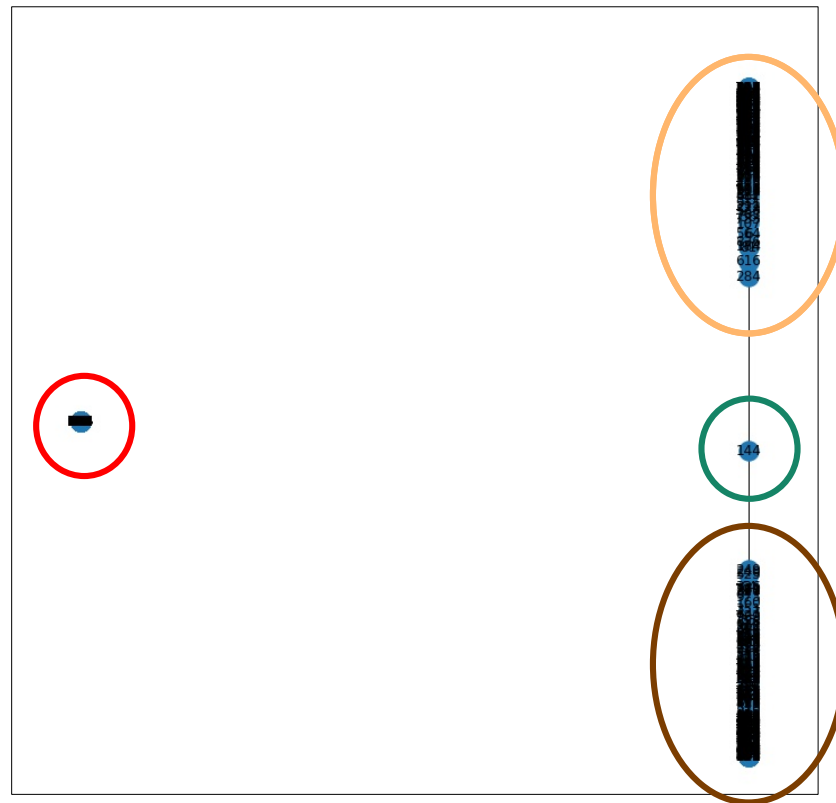
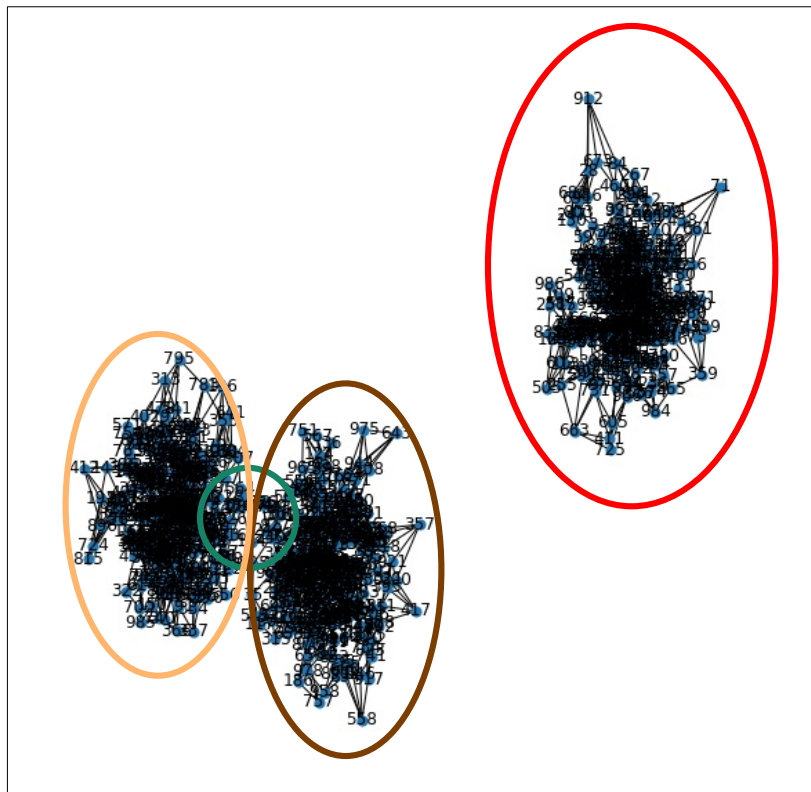
```
nx.draw_spectral(G, with_labels=True)
```





# 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