## Spectral Graph Embedding

#### Social Networks Analysis and Graph Algorithms

Prof. Carlos Castillo — <a href="https://chato.cl/teach">https://chato.cl/teach</a>



#### Sources

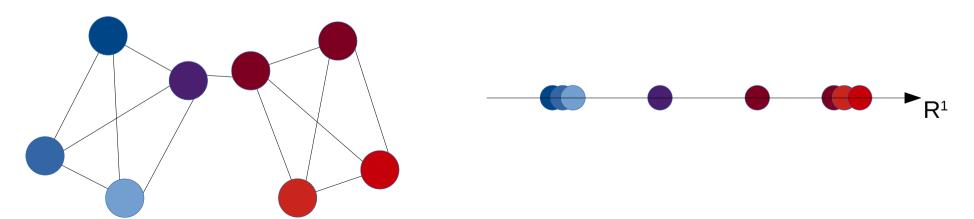
- J. Leskovec (2016). Defining the graph laplacian [video]
- E. Terzi (2013). Graph cuts The part on spectral graph partitioning
- D. A. Spielman (2009): The Laplacian
- URLs cited in the footer of slides

## Many algorithms are not suitable for graphs

- Many algorithms need a notion of similarity or distance (both are interchangeable)
- Data mining: clustering, outlier detection, ...
- Retrieval/search: nearest neighbors, ...

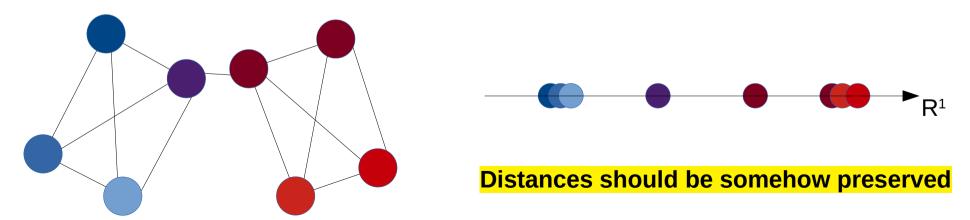
## Graphs are nice, but ...

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



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## 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, ..., 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?



## 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

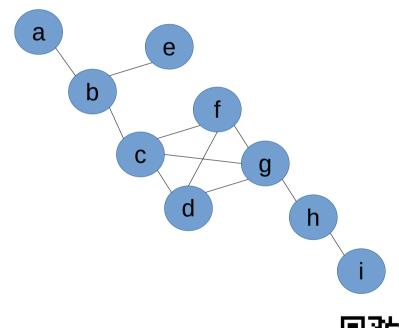
## Random graph projection (2D)

- 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<sub>i</sub>, y<sub>i</sub>)

## **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
- ullet Draw the graph in an  $\mathbb{R}^2$  plane lacktriangle







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

# Refresher about eigenvectors/eigenvalues

## Eigenvectors of symmetric matrices

- In general  $Av = \lambda v$  means A has an eigenvector v of eigenvalue  $\lambda$
- In symmetric matrices  $(A=A^T)$ , eigenvectors are orthogonal Suppose  $v_1$ ,  $v_2$  are eigenvectors of eigenvalues  $\lambda_1$ ,  $\lambda_2$  with  $\lambda_1 \neq \lambda_2$

$$\lambda_1 \langle v_1, v_2 \rangle = \langle \lambda_1 v_1, v_2 \rangle = \langle A v_1, v_2 \rangle = \langle v_1, A^T v_2 \rangle$$
 For any real matrix 
$$= \langle v_1, A v_2 \rangle = \langle v_1, \lambda_2 v_2 \rangle = \lambda_2 \langle v_1, v_2 \rangle$$
 
$$\langle A x, y \rangle = \langle x, A^T y \rangle$$

• Therefore:

$$(\lambda_1 - \lambda_2) \langle v_1, v_2 \rangle = 0 \wedge (\lambda_1 - \lambda_2) \neq 0 \Rightarrow \langle v_1, v_2 \rangle = 0$$

## 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 smallest eigenvalue is

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

# Eigenvectors of the adjacency matrix (of an unweighted graph)

## Adjacency matrix (of unweighted graph)

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

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:

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ a_{21} & \dots & a_{2n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \qquad \begin{aligned} y_i &= \sum_{j:(j,i) \in E} x_j \\ \vdots \\ y_n \end{bmatrix}$$

$$\begin{bmatrix} x_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$
Ax is a vector whose i<sup>th</sup> coordinate contains the sum of

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

coordinate contains the sum of the  $x_i$  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:  $k_i = d \ \forall i$
- Multiply its adjacency by 1
- 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

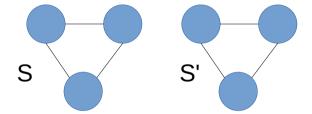
• Suppose graph is d-regular, i.e. all nodes have degree d:

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

• Hence,  $[1, 1, ..., 1]^T$  is an eigenvector of eigenvalue d

## Disconnected graphs

Suppose the graph is regular and disconnected

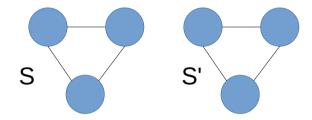


Then its adjacency matrix has block structure:

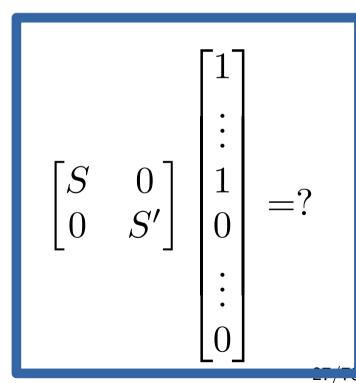
$$A = \begin{bmatrix} S & 0 \\ 0 & S' \end{bmatrix}$$

## Disconnected graphs

Suppose the graph is regular and disconnected

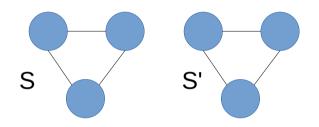


Let 
$$x_i^S = \begin{cases} 1 & \text{if } i \in S \\ 0 & \text{if } i \in S' \end{cases}$$



## Disconnected graphs

Suppose the graph is regular and disconnected



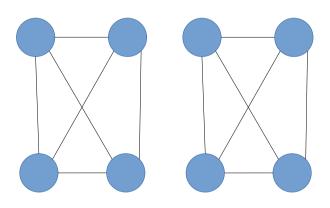
$$Ax^S = dx^S$$

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

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

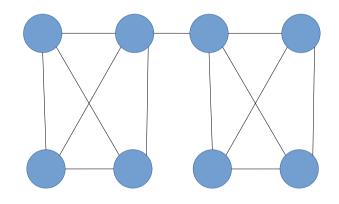
## In general

Disconnected graph



$$\lambda_1 = \lambda_2$$

Almost disconnected graph



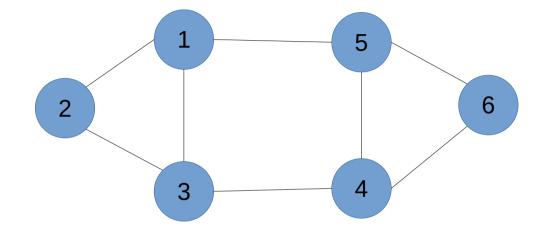
$$\lambda_1 \approx \lambda_2$$

Small "eigengap"

## **Graph Laplacian**

## Adjacency matrix

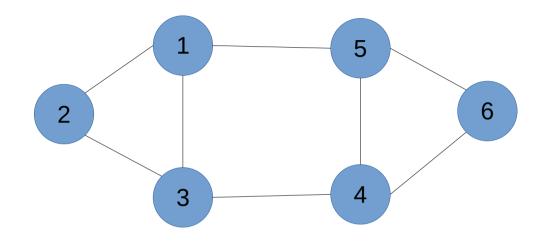
$$A_{ij} = \begin{cases} 1 & \text{if } (i,j) \in E \\ 0 & \text{otherwise} \end{cases}$$



	Įυ	T	T	U	1	υĮ
A =	1	0	1	0	0	0
	1	1	0	1	0	0
	0	0	1	0	1	1
	1	0	0	0 1 0 1 1	0	1
	0	0	0	1	1	$\begin{bmatrix} 1 \\ 0 \end{bmatrix}$
	_					32

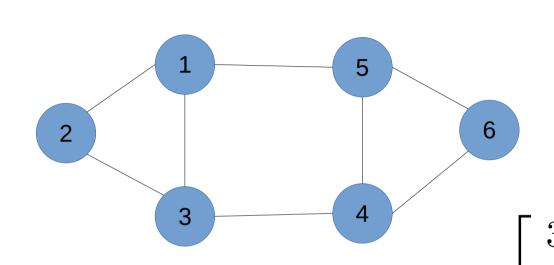
## Degree matrix

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



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

## Laplacian matrix



L = D - A

 $L = \begin{bmatrix} -1 & -1 & 3 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ -1 & 0 & 0 & -1 & 3 & -1 \\ 0 & 0 & 0 & -1 & 3 & -1 \end{bmatrix}$  Given A is symmetric. They only differ in the diagonal.

## Laplacian matrix L = D - A

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

## The constant vector is an eigenvector of L

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

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

Does it need to be this specific graph? Why?

Does it need to be the vector [1, 1, ..., 1]? 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 
$$\mathbf{x}^T L \mathbf{x} = \sum_{(i,j) \in E} (x_i - x_j)^2$$

$$L_{ij} = D_{ij} - A_{ij}$$

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

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

## As shown before, the constant vector is one of the eigenvectors of L, with eigenvalue 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 the constant vector is an eigenvector of L with eigenvalue 0

## The eigenvector x of $\lambda = 0$ is the constant vector if the graph is connected

• If x is the eigenvector of eigenvalue 0, Lx = 0

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

From this, we deduct that  $x_i = x_j$  for any pair i, j even if i and j are not directly connected by an edge. Why?

# The eigenvector x of $\lambda = 0$ is the constant vector if the graph is connected

- If x is the eigenvector of eigenvalue 0, Lx = 0
- Then  $x^T L x = \sum_{(i,j) \in E} (x_i x_j)^2 = 0$
- Hence, for any pair of nodes (i,j) connected by an edge,  $x_i = x_j$
- Given the graph is connected, there is a path between any two nodes  $\Rightarrow$  for any pair of nodes (i,j), even the ones not connected by an edge,  $x_i = x_j$
- Hence x is a constant vector

# All the eigenvalues of the Laplacian are non-negative

• If  $\nu$  is an eigenvector of L of eigenvalue  $\lambda$ :

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

• This means all eigenvalues  $\lambda$  are non-negative

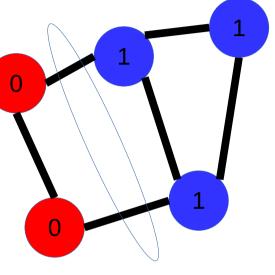
# In summary, the Laplacian matrix L = D - A

- Is symmetric, eigenvectors are orthogonal
- ullet Has N eigenvalues that are non-negative
- 0 is one eigenvalue  $0 = \lambda_1 \le \lambda_2 \le ... \le \lambda_N$
- $^{ullet}$  The multiplicity of eigenvalue O equals the number of connected components of the graph

# The second smallest eigenvalue of the Laplacian

# x<sup>T</sup>Lx and graph cuts

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



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

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

#### Remember

For symmetric matrices

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

• If x is an eigenvector,  $\frac{x^T M x}{x^T x}$  is its eigenvalue

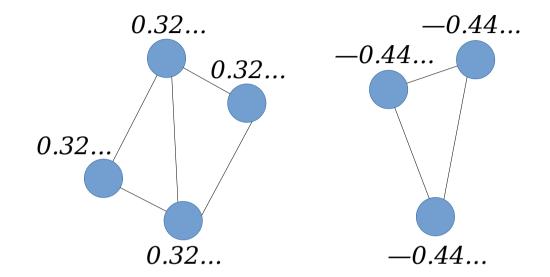
# Second eigenvector

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

$$\lambda_2 = \min_{x} \frac{x^T L x}{x^T x} = \min_{x: \sum x_i = 0} \frac{x^T L x}{\sum x_i^2} = \min_{x: \sum x_i = 0 \land \sum x_i^2 = 1} \sum_{(i,j) \in E} (x_i - x_j)^2$$

# The second eigenvalue in a disconnected graph

If the graph is divided into two connected components of sizes  $N_1$  and  $N_2$ , you can use this assignment

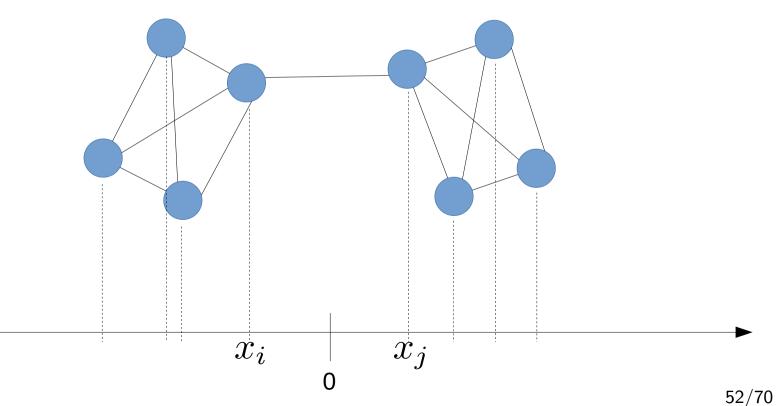


$$\lambda_2 = \min_{x: \sum x_i = 0 \land \sum x_i^2 = 1} \sum_{(i,j) \in E} (x_i - x_j)^2$$

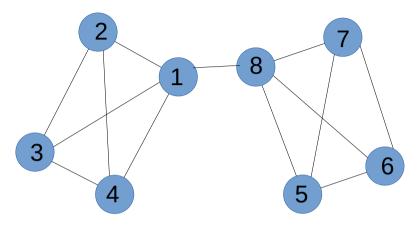
# The second eigenvalue tells us how well the graph can be partitioned into two

$$\lambda_2 = \min_{x: \sum x_i = 0 \land \sum x_i^2 = 1} \sum_{(i,j) \in E} (x_i - x_j)^2$$

If the graph is connected but almost partitioned into two component, the optimal X should have values similar to each other in each partition

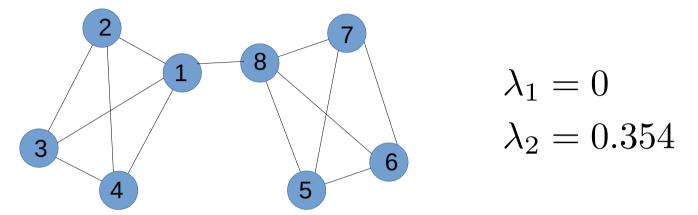


#### Example Graph 1



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

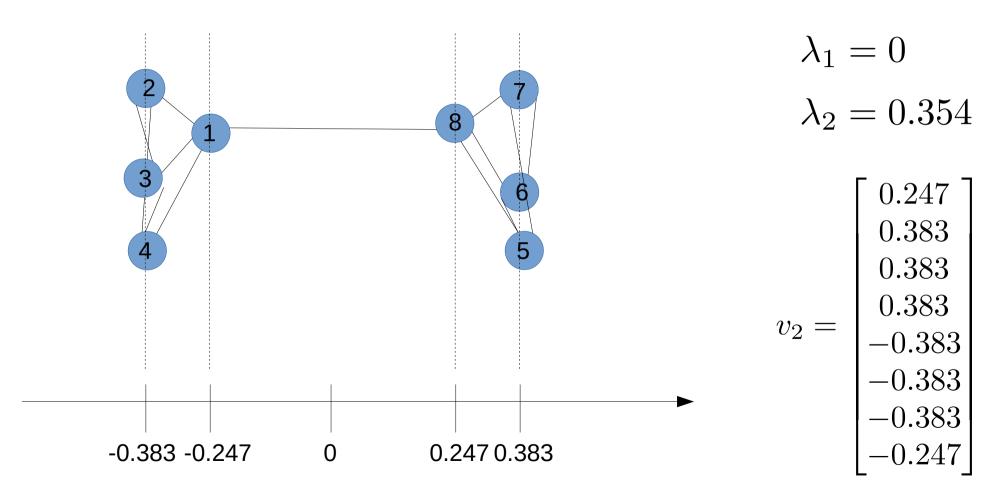
## Example Graph 1 (second eigenvalue of L)



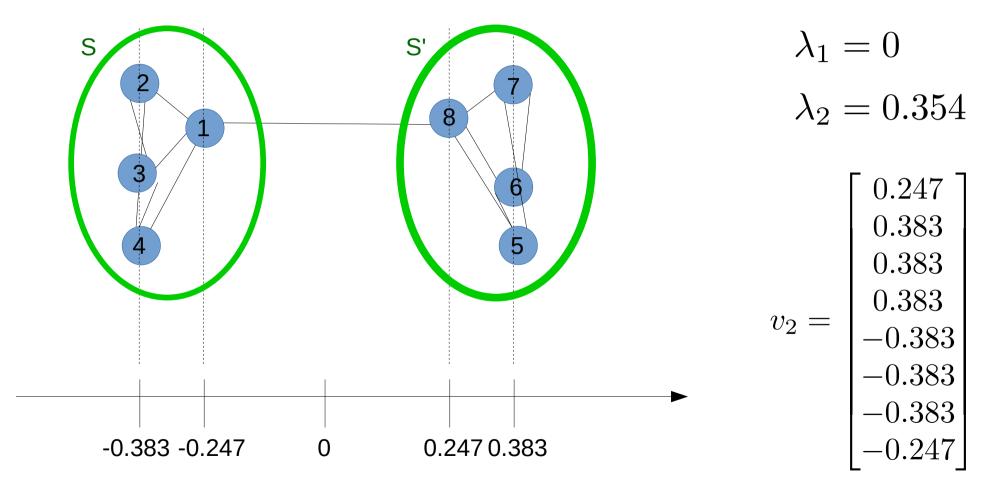
$$L = \begin{bmatrix} -1 & 3 & -1 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 3 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & -1 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & -1 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 3 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & -1 & 3 & -1 \\ -1 & 0 & 0 & 0 & -1 & -1 & -1 & 4 \end{bmatrix}$$

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

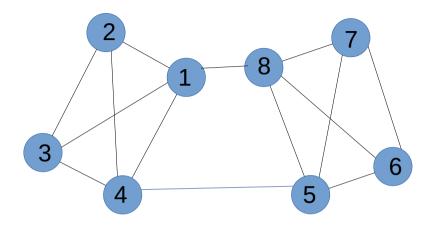
# Example Graph 1, projected in R<sup>1</sup>



# Example Graph 1, communities

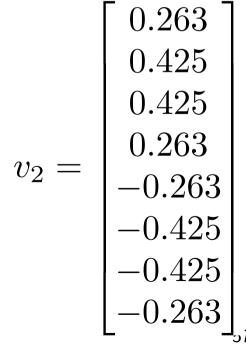


# Example Graph 2

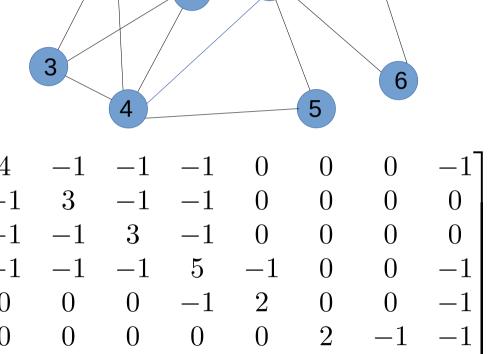


$$\begin{bmatrix} 4 & -1 & -1 & -1 & 0 & 0 & 0 & -1 \\ -1 & 3 & -1 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 3 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & -1 & 4 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 4 & -1 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 3 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & -1 & 3 & -1 \\ -1 & 0 & 0 & 0 & -1 & -1 & -1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

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

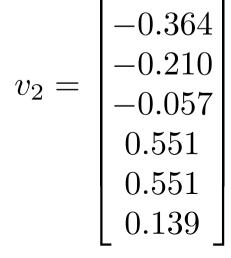


# Example Graph 3

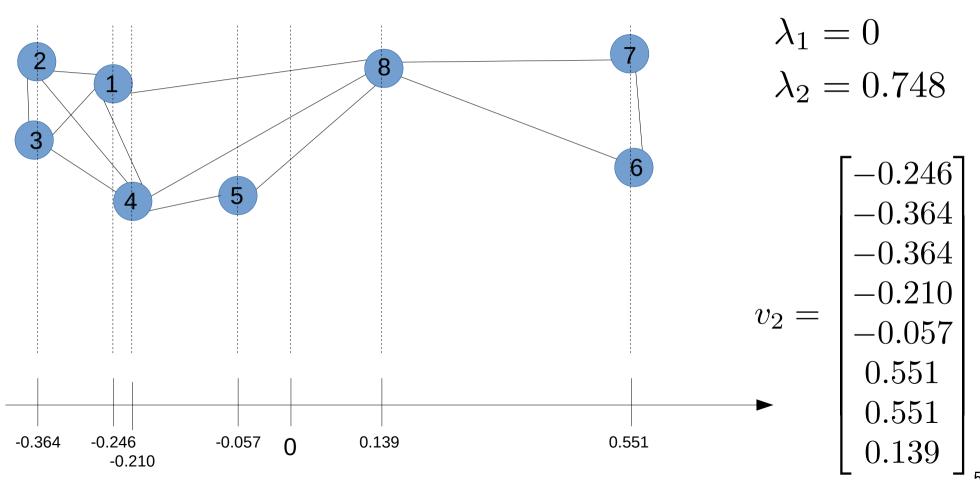


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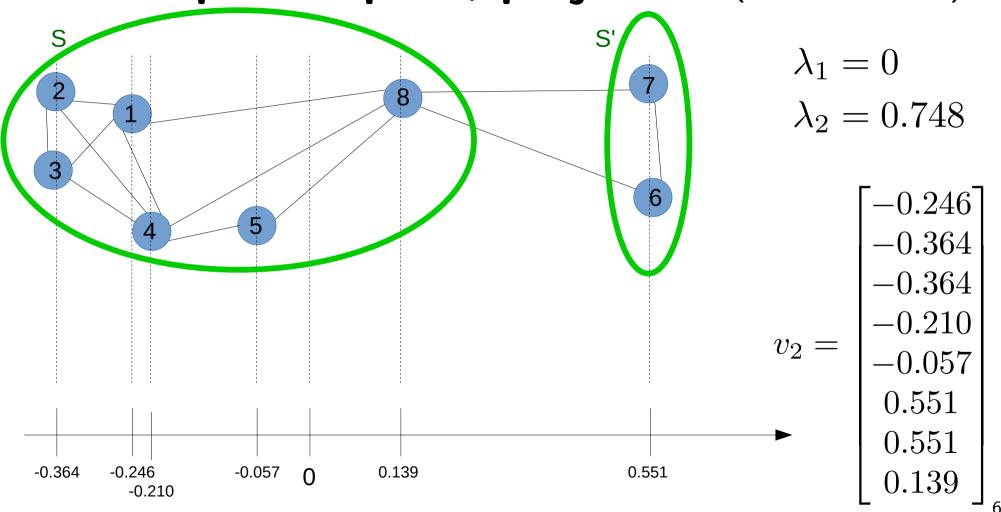
$$\lambda_1 = 0$$
$$\lambda_2 = 0.748$$



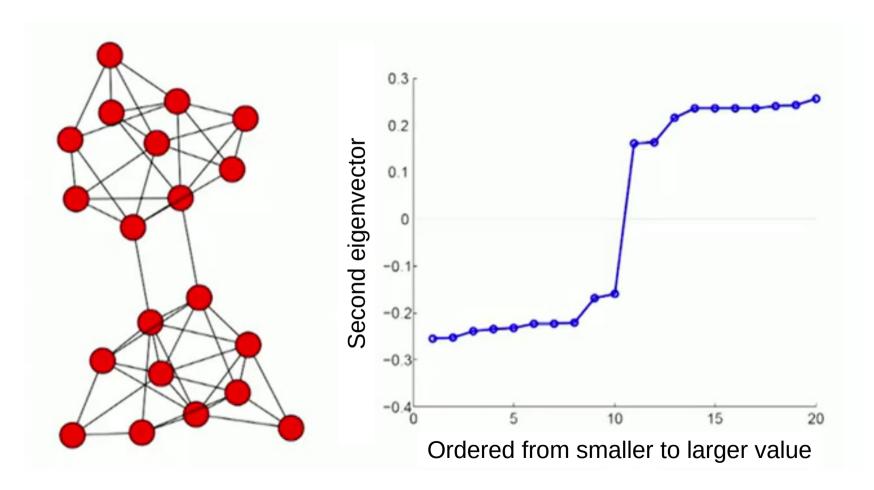
#### Example Graph 3, projected (where to cut?)



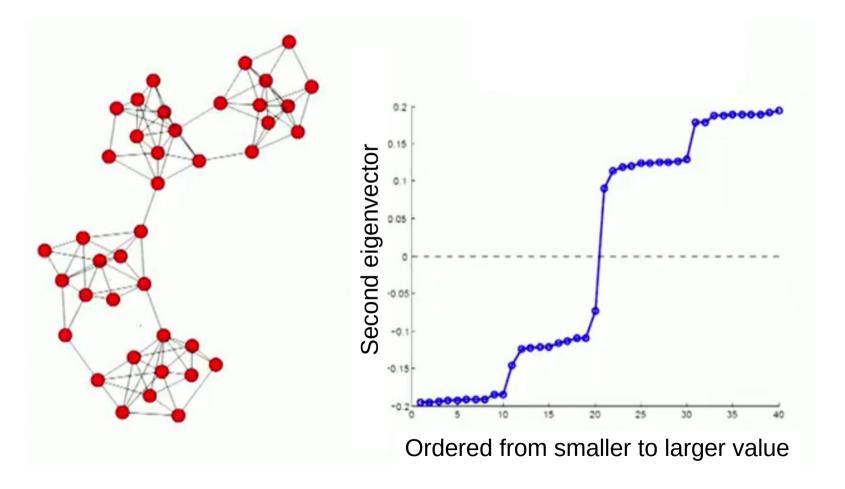
#### Example Graph 3, projected (where to cut?)



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

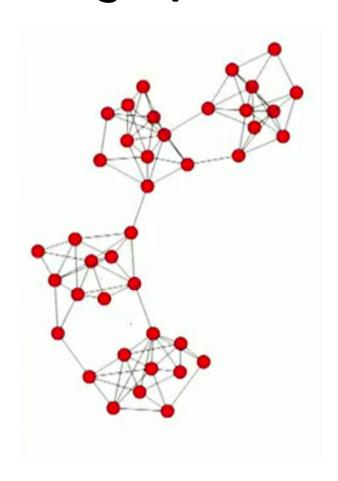


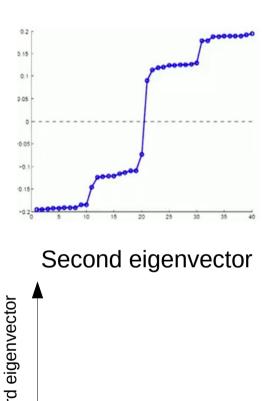
# A graph with four communities in $\mathbb{R}^1$

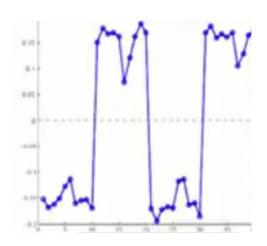


# Application: graph drawing

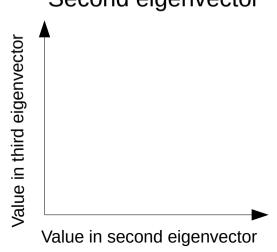
# A graph with four communities in $\mathbb{R}^2$



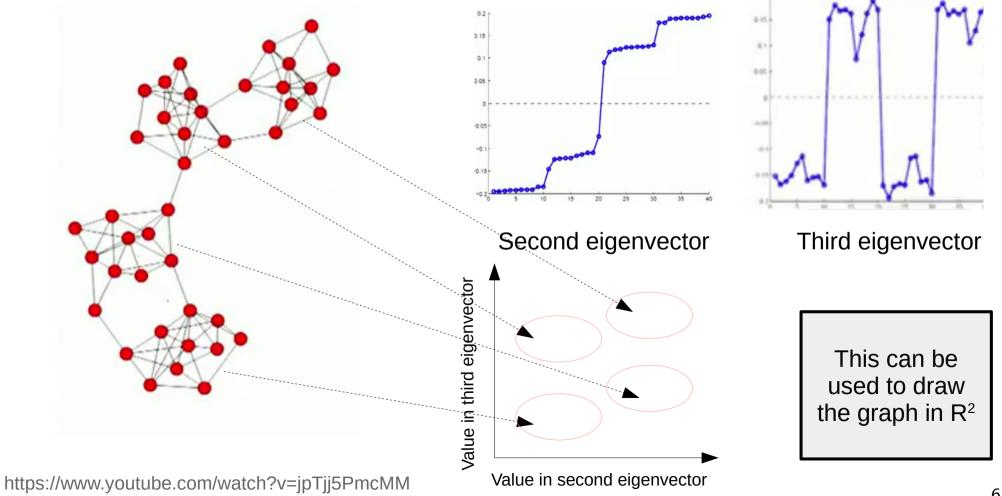




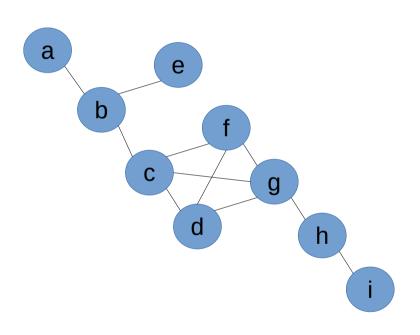
Third eigenvector



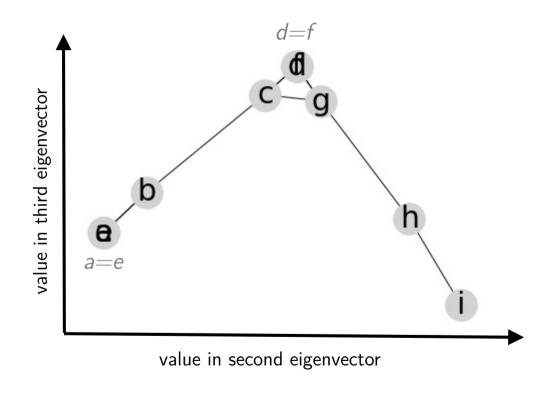
# A graph with four communities in R<sup>2</sup> (cont)



#### The graph from the initial exercise



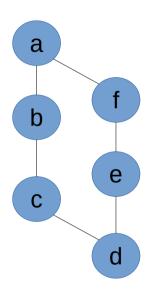
Input nodes and edges



Spectral embedding

## **Exercise:** spectral projection

- Write the Laplacian
- Get the second and third eigenvector (e.g., "online eigenvector calculator")
- Obtain projection



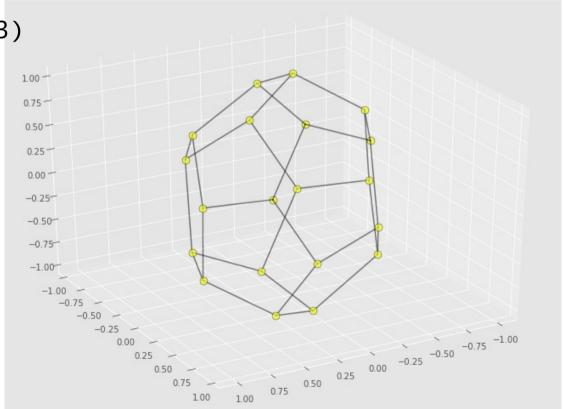


# A barbell graph in R<sup>2</sup> (code)

```
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

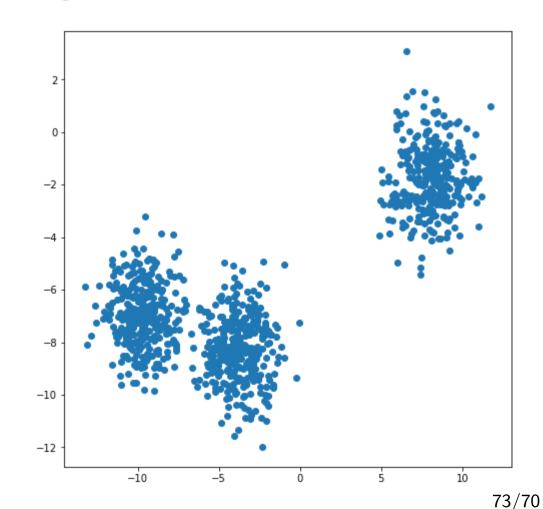
g = nx.dodecahedral\_graph()
pos = nx.spectral\_layout(g, dim=3)
network\_plot\_3D\_alt(g, 60, pos)



# **Application:** spectral clustering

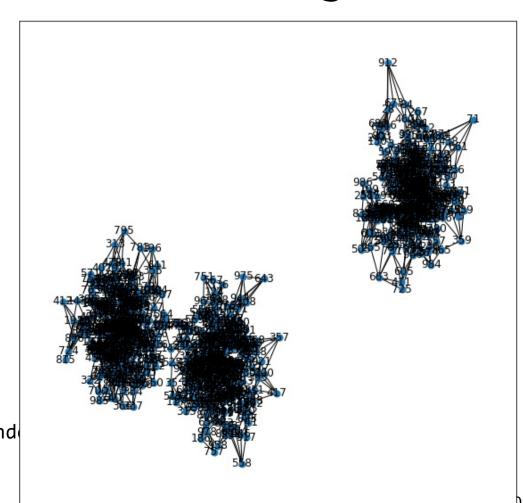
## **Generating data**

```
from sklearn.datasets import
   make blobs
  = 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()
```



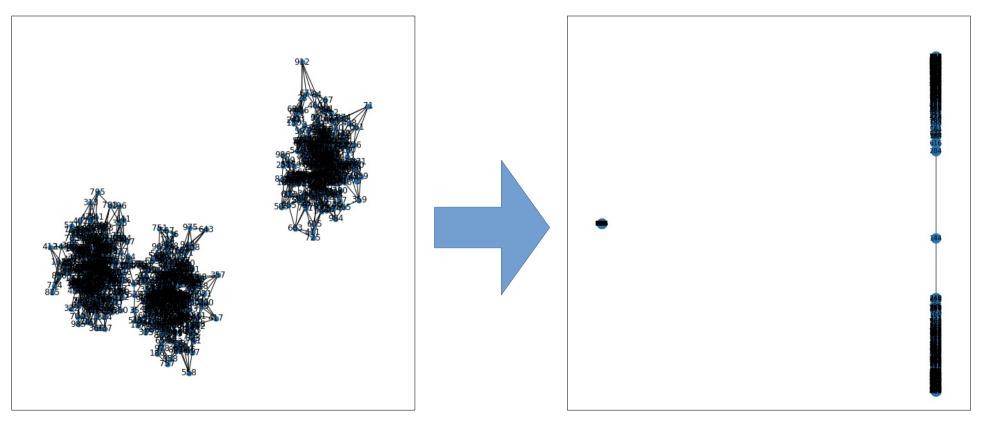
# Connect nodes to k=5 nearest neighbors

```
from sklearn.neighbors
  import NearestNeighbors
nbrs = NearestNeighbors(
   .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 ind
       G.add edge(source node, target node)
```



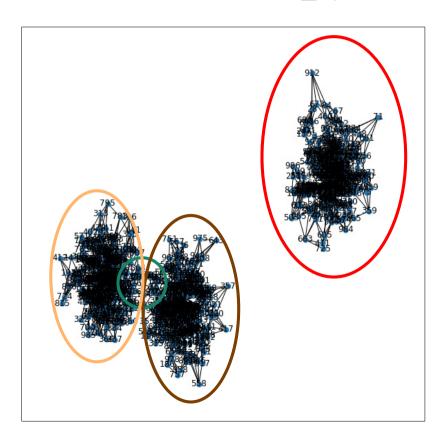
# Perform spectral embedding

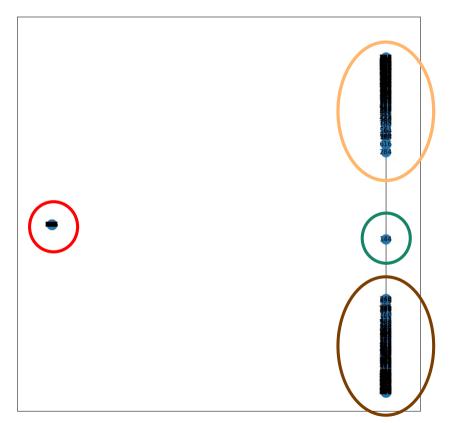
nx.draw\_spectral(G, with\_labels=True)



# 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