## Spectral Graph Embedding

Social Networks Analysis and Graph Algorithms
Prof. Carlos Castillo - https://chato.cl/teach

## 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
- We will try to transform a graph into a more familiar object: a cloud of points in $\mathrm{R}^{\mathrm{k}}$



## 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 $\mathrm{R}^{k}$


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

$$
\begin{aligned}
V= & \{v 1, v 2, \ldots, v 8\} \\
E= & \{(v 1, v 2),(v 2, v 3),(v 3, v 4),(v 4, v 1),(v 5, v 6),(v 6, v 7),(v 7, v 8), \\
& (v 8, v 5),(v 1, v 5),(v 2, v 6),(v 3, v 7),(v 4, v 8)\}
\end{aligned}
$$

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 $\mathrm{y}=1$, and nodes visited have ascending y
- Project node i to position $\left(\mathrm{x}_{\mathrm{i}}, \mathrm{y}_{\mathrm{i}}\right)$


## Exercise: random projection

- Given this graph
- Pick a random node $u$
- Distances from $u$ are the $\times$ positions
- Pick a random node v

- Distances from $v$ are the $y$ positions
- Draw the graph in an $\mathbb{R}^{2}$ plane


## Refresher about

## eigenvectors/eigenvalues

## Eigenvectors of symmetric matrices

- In general $A v=\lambda v$ means $A$ has an eigenvector $v$ of eigenvalue $\lambda$
- In symmetric matrices $\left(A=A^{T}\right)$, eigenvectors are orthogonal Suppose $\nu_{1}, \nu_{2}$ are eigenvectors of eigenvalues $\lambda_{1}, \lambda_{2}$ with $\lambda_{1} \neq \lambda_{2}$

$$
\begin{aligned}
\lambda_{1}\left\langle v_{1}, v_{2}\right\rangle & =\left\langle\lambda_{1} v_{1}, v_{2}\right\rangle=\left\langle A v_{1}, v_{2}\right\rangle=\left\langle v_{1}, A^{T} v_{2}\right\rangle & & \text { For any real matrix } \\
& =\left\langle v_{1}, A v_{2}\right\rangle=\left\langle v_{1}, \lambda_{2} v_{2}\right\rangle=\lambda_{2}\left\langle v_{1}, v_{2}\right\rangle & & \langle A x, y\rangle=\left\langle x, A^{T} y\right\rangle
\end{aligned}
$$

- Therefore:

$$
\left(\lambda_{1}-\lambda_{2}\right)\left\langle v_{1}, v_{2}\right\rangle=0 \wedge\left(\lambda_{1}-\lambda_{2}\right) \neq 0 \Rightarrow\left\langle v_{1}, v_{2}\right\rangle=0
$$

## 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)

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

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

$$
\left[\begin{array}{ccc}
a_{11} & \cdots & a_{1 n} \\
a_{21} & \cdots & a_{2 n} \\
\vdots & \ddots & \vdots \\
a_{n 1} & \cdots & a_{n n}
\end{array}\right]
$$

## Adjacency matrix of $G=(\mathrm{V}, \mathrm{E})$

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

## Can you write $\boldsymbol{y}_{i}$ using $\boldsymbol{E}$ ?

$$
\left[\begin{array}{ccc}
a_{11} & \cdots & a_{1 n} \\
a_{21} & \cdots & a_{2 n} \\
\vdots & \ddots & \vdots \\
a_{n 1} & \cdots & a_{n n}
\end{array}\right]\left[\begin{array}{c}
x_{1} \\
x_{2} \\
\vdots \\
x_{n}
\end{array}\right]=\left[\begin{array}{c}
y_{1} \\
y_{2} \\
\vdots \\
y_{n}
\end{array}\right]
$$

## Adjacency matrix of $\mathrm{G}=(\mathrm{V}, \mathrm{E})$

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

- What is $\boldsymbol{A x}$ ? Think of $\chi$ as a set of labels/values:
$\left[\begin{array}{ccc}a_{11} & \cdots & a_{1 n} \\ a_{21} & \cdots & a_{2 n} \\ \vdots & \ddots & \vdots \\ a_{n 1} & \cdots & a_{n n}\end{array}\right]\left[\begin{array}{c}x_{1} \\ x_{2} \\ \vdots \\ x_{n}\end{array}\right]=\left[\begin{array}{c}y_{1} \\ y_{2} \\ \vdots \\ y_{n}\end{array}\right]$

$$
y_{i}=\sum_{j:(i, j) \in E} x_{j}
$$

$A x$ is a vector whose $\mathrm{ith}^{\text {th }}$ coordinate contains the sum of the $\mathrm{x}_{\mathrm{j}}$ who are in-neighbors of i

## Spectral graph theory ...

- Studies the eigenvalues and eigenvectors of a graph matrix
- Adjacency matrix $A x=\lambda x$
- Laplacian matrix (next)
- Suppose graph is d-regular: $k_{i}=d \forall i$
- Multiply its adjacency by $\mathbf{1}^{-}$
- Look at the result, what does it imply?

$$
\left[\begin{array}{ccc}
a_{11} & \cdots & a_{1 n} \\
a_{21} & \cdots & a_{2 n} \\
\vdots & \ddots & \vdots \\
a_{n 1} & \cdots & a_{n n}
\end{array}\right]\left[\begin{array}{c}
1 \\
1 \\
\vdots \\
1
\end{array}\right]=?
$$

## An eigenvector of a d-regular graph

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

$$
\left[\begin{array}{ccc}
a_{11} & \cdots & a_{1 n} \\
a_{21} & \ldots & a_{2 n} \\
\vdots & \ddots & \vdots \\
a_{n 1} & \cdots & a_{n n}
\end{array}\right]\left[\begin{array}{c}
1 \\
1 \\
\vdots \\
1
\end{array}\right]=\left[\begin{array}{c}
d \\
d \\
\vdots \\
d
\end{array}\right]=d\left[\begin{array}{c}
1 \\
1 \\
\vdots \\
1
\end{array}\right]
$$

- Hence, $[1,1, \ldots, 1]^{\top}$ is an eigenvector of eigenvalue d


## Disconnected graphs

- Suppose the graph is regular and disconnected

- Then its adjacency matrix has block structure:

$$
A=\left[\begin{array}{cc}
S & 0 \\
0 & S^{\prime}
\end{array}\right]
$$

## Disconnected graphs

- Suppose the graph is regular and disconnected


S S'

$$
\left[\begin{array}{cc}
S & 0 \\
0 & S^{\prime}
\end{array}\right]\left[\begin{array}{c}
1 \\
0 \\
\vdots \\
0
\end{array}\right]=?
$$

## Disconnected graphs

- Suppose the graph is regular and disconnected


S


$$
\begin{aligned}
A x^{S} & =d x^{S} \\
A x^{S^{\prime}} & =d x^{S^{\prime}}
\end{aligned}
$$

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



# Degree matrix 

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



## Laplacian matrix

$$
L=D-A
$$

Because A is symmetric, and we have only changed the diagonal, $L$ is symmetric.

$$
L=\left[\begin{array}{cccccc}
3 & -1 & -1 & 0 & -1 & 0 \\
-1 & 2 & -1 & 0 & 0 & 0 \\
-1 & -1 & 3 & -1 & 0 & 0 \\
0 & 0 & -1 & 3 & -1 & -1 \\
-1 & 0 & 0 & -1 & 3 & -1 \\
0 & 0 & 0 & -1 & -1 & 2
\end{array}\right.
$$

## Laplacian matrix $L=D-A$

$$
L \overrightarrow{1}=\left[\begin{array}{cccccc}
3 & -1 & -1 & 0 & -1 & 0 \\
-1 & 2 & -1 & 0 & 0 & 0 \\
-1 & -1 & 3 & -1 & 0 & 0 \\
0 & 0 & -1 & 3 & -1 & -1 \\
-1 & 0 & 0 & -1 & 3 & -1 \\
0 & 0 & 0 & -1 & -1 & 2
\end{array}\right]\left[\begin{array}{l}
1 \\
1 \\
1 \\
1 \\
1 \\
1
\end{array}\right]=?
$$

## The constant vector is an eigenvector of $L$

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

$$
L x=\left[\begin{array}{cccccc}
3 & -1 & -1 & 0 & -1 & 0 \\
-1 & 2 & -1 & 0 & 0 & 0 \\
-1 & -1 & 3 & -1 & 0 & 0 \\
0 & 0 & -1 & 3 & -1 & -1 \\
-1 & 0 & 0 & -1 & 3 & -1 \\
0 & 0 & 0 & -1 & -1 & 2
\end{array}\right]\left[\begin{array}{l}
1 \\
1 \\
1 \\
1 \\
1 \\
1
\end{array}\right]=\left[\begin{array}{l}
0 \\
0 \\
0 \\
0 \\
0 \\
0
\end{array}\right]=0\left[\begin{array}{l}
1 \\
1 \\
1 \\
1 \\
1 \\
1
\end{array}\right]
$$

Does it need to be this specific graph? Why?
Does it need to be the vector $[1,1, \ldots, 1]$ ? 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 $\mathrm{x}^{T} L x=\sum_{(i, j) \in E}\left(x_{i}-x_{j}\right)^{2}$

$$
\begin{aligned}
L_{i j} & =D_{i j}-A_{i j} \\
D_{i j} & =\left\{\begin{array}{ll}
k_{i} & \text { if } i=j \\
0 & \text { otherwise }
\end{array} \quad A_{i j}= \begin{cases}1 & \text { if }(i, j) \in E \\
0 & \text { otherwise }\end{cases} \right.
\end{aligned}
$$

Assume that E only contains each edge in one direction
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 $\chi$ is such that $X_{i}=\chi_{j}$ for all $i, j$ :

$$
x^{T} L x=\sum_{(i, j) \in E}\left(x_{i}-x_{j}\right)^{2}=0 \Rightarrow L x=0
$$

- 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 $0, L x=0$
- Then $x^{T} L x=\sum_{(i, j) \in E}\left(x_{i}-x_{j}\right)^{2}=0$

From this, we deduct that $\chi_{i}=\chi_{j}$ 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 $0, L x=0$
- Then $x^{T} L x=\sum_{(i, j) \in E}\left(x_{i}-x_{j}\right)^{2}=0$
- Hence, for any pair of nodes ( $i, j$ ) connected by an edge, $\chi_{i}=\chi_{j}$
- 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 $v$ is an eigenvector of $L$ of eigenvalue $\lambda$ :

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

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


## In summary, the Laplacian matrix $\mathrm{L}=\mathrm{D}-\mathrm{A}$

- Is symmetric, eigenvectors are orthogonal
- Has $N$ eigenvalues that are non-negative
- 0 is one eigenvalue $0=\lambda_{1} \leq \lambda_{2} \leq \ldots \leq \lambda_{N}$
- The multiplicity of eigenvalue 0 equals the number of connected components of the graph


## The second smallest eigenvalue of the Laplacian

## $x^{\top} L x$ and graph cuts

- Suppose $c\left(S, S^{\prime}\right)$ is a cut of graph $G$
- Set $x_{i}= \begin{cases}1 & \text { if } i \in S \\ 0 & \text { if } i \in S^{\prime}\end{cases}$


$$
\left|c\left(S, S^{\prime}\right)\right|=2
$$

$$
x^{T} L x=\sum_{(i, j) \in E}\left(x_{i}-x_{j}\right)^{2}=\sum_{(i, j) \in c\left(S, S^{\prime}\right)} 1^{2}=\left|c\left(S, S^{\prime}\right)\right|
$$

## Remember

- For symmetric matrices

$$
\lambda_{2}=\min _{x} \frac{x^{T} M x}{x^{T} x}
$$

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


## Second eigenvector

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

$$
\lambda_{2}=\min _{x} \frac{x^{T} L x}{x^{T} x}=\min _{x: \sum x_{i}=0} \frac{x^{T} L x}{\sum x_{i}^{2}}=\min _{x: \sum x_{i}=0 \wedge \sum x_{i}^{2}=1} \sum_{(i, j) \in E}\left(x_{i}-x_{j}\right)^{2}
$$

## 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

What's its eigenvalue?

$$
\lambda_{2}=\min _{x: \sum x_{i}=0 \wedge \sum x_{i}^{2}=1} \sum_{(i, j) \in E}\left(x_{i}-x_{j}\right)^{2}
$$

## The second eigenvalue tells us

## how well the graph can be partitioned into two

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

$$
\lambda_{2}=\min _{x: \sum x_{i}=0 \wedge \sum x_{i}^{2}=1} \sum_{(i, j) \in E}\left(x_{i}-x_{j}\right)^{2}
$$



## Example Graph 1



## Example Graph 1 (second eigenvalue of $L$ )



$$
L=\left[\begin{array}{cccccccc}
4 & -1 & -1 & -1 & 0 & 0 & 0 & -1 \\
-1 & 3 & -1 & -1 & 0 & 0 & 0 & 0 \\
-1 & -1 & 3 & -1 & 0 & 0 & 0 & 0 \\
-1 & -1 & -1 & 3 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 3 & -1 & -1 & -1 \\
0 & 0 & 0 & 0 & -1 & 3 & -1 & -1 \\
0 & 0 & 0 & 0 & -1 & -1 & 3 & -1 \\
-1 & 0 & 0 & 0 & -1 & -1 & -1 & 4
\end{array}\right] \quad v_{2}=\left[\begin{array}{c}
0.247 \\
0.383 \\
0.383 \\
0.383 \\
-0.383 \\
-0.383 \\
-0.383 \\
-0.247
\end{array}\right]
$$

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



## Example Graph 1, communities



## Example Graph 2

$$
\begin{aligned}
& L=\left[\begin{array}{cccccccc}
4 & -1 & -1 & -1 & 0 & 0 & 0 & -1 \\
-1 & 3 & -1 & -1 & 0 & 0 & 0 & 0 \\
-1 & -1 & 3 & -1 & 0 & 0 & 0 & 0 \\
-1 & -1 & -1 & 4 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 4 & -1 & -1 & -1 \\
0 & 0 & 0 & 0 & -1 & 3 & -1 & -1 \\
0 & 0 & 0 & 0 & -1 & -1 & 3 & -1 \\
-1 & 0 & 0 & 0 & -1 & -1 & -1 & 4
\end{array}\right] \\
& \lambda_{1}=0 \\
& \lambda_{2}=0.764
\end{aligned}
$$

## Example Graph 3



$$
L=\left[\begin{array}{cccccccc}
4 & -1 & -1 & -1 & 0 & 0 & 0 & -1 \\
-1 & 3 & -1 & -1 & 0 & 0 & 0 & 0 \\
-1 & -1 & 3 & -1 & 0 & 0 & 0 & 0 \\
-1 & -1 & -1 & 5 & -1 & 0 & 0 & -1 \\
0 & 0 & 0 & -1 & 2 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 & 2 & -1 & -1 \\
0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 \\
-1 & 0 & 0 & -1 & -1 & -1 & -1 & 5
\end{array}\right] \quad v_{2}=\left[\begin{array}{c}
-0.364 \\
-0.364 \\
-0.210 \\
-0.057 \\
0.551 \\
0.551 \\
0.139
\end{array}\right]
$$

## 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 $\mathbb{R}^{1}$

Note the hierarchical community structure


Ordered from smaller to larger value

# Application: graph drawing 

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




Second eigenvector


Third eigenvector

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




Second eigenvector



Third eigenvector

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

## The graph from the initial exercise



Input nodes and edges


Spectral embedding

## Exercise: spectral projection

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


## A barbell graph in $\mathrm{R}^{2}$ (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
$\mathrm{N}=1000$

plt.figure(figsize=(8,8))
plt.scatter(x[:,0], x[:,1])
plt.show()


## Connect nodes to $\mathrm{k}=5$ 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(ne\overline{ighbor_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

