Spectral Graph Embedding

Social Networks Analysis and Graph Algorithms

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



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 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?





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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 lacksquare





Refresher about eigenvectors/eigenvalues

Eigenvectors of symmetric matrices

- In general $Av = \lambda v$ means A has an eigenvector v of eigenvalue λ
- In symmetric matrices (A=A^T), eigenvectors are orthogonal
 Suppose ν₁, ν₂ are eigenvectors of eigenvalues λ₁, λ₂ with λ₁ ≠ λ₂

$$\begin{split} \lambda_1 \langle v_1, v_2 \rangle &= \langle \lambda_1 v_1, v_2 \rangle = \langle A v_1, v_2 \rangle = \langle v_1, A^T v_2 \rangle & \quad \text{For any real matrix} \\ &= \langle v_1, A v_2 \rangle = \langle v_1, \lambda_2 v_2 \rangle = \lambda_2 \langle v_1, v_2 \rangle & \quad \langle A x, y \rangle = \langle x, A^T y \rangle \end{split}$$

• Therefore:

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

In symmetric matrices

- The multiplicity of an eigenvalue λ is the dimension of the space of eigenvectors of eigenvalue λ
- Every *n* x *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

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

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

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?

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

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

Adjacency matrix of G=(V,E)

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



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

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

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

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

Ax is a vector whose i^{th} 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
- Look at the result, what does it 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





Disconnected graphs

• Suppose the graph is regular and disconnected



- 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







Laplacian matrix L = D - A



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



Prove this!

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

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

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

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

 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, 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, jeven 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 v is an eigenvector of L of eigenvalue λ :

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

• This means all eigenvalues λ are non-negative

In summary, the Laplacian matrix L = D - A

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

The second smallest eigenvalue of the Laplacian

$\mathbf{x}^{\mathsf{T}}\mathbf{L}\mathbf{x}$ and graph cuts

- Suppose c(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

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

Second eigenvector

• Orthogonal to the first one: $x \cdot \vec{1} = 0 \Rightarrow \sum x_i = 0$

• 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

What's its eigenvalue?



 $\lambda_2 = \min_{x:\sum x_i = 0 \land \sum x_i^2 = 1} \sum_{(i,j) \in E} (x_i - x_j)^2$ 51/70

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



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

Example Graph 1 (second eigenvalue of L)



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

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

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Example Graph 1, projected in R¹



Example Graph 1, communities





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Example Graph 3, projected (where to cut?)





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



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

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



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

Application: graph drawing

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







A graph with four communities in R² (cont)



The graph from the initial exercise



value in second eigenvector

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





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



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
```

```
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