Lecture 11: Introduction to Spectral Graph Theory

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We will start *spectral graph theory* from these lecture notes. The main objective of spectral graph theory is to relate properties of graphs with the eigenvalues and eigenvectors (spectral properties) of *associated* matrices.

These lecture notes will talk about various matrices which can be associated with a graph, like adjacency, edge adjacency and Laplacian matrix. The connection between these matrices will be explored.

We will also introduce a quadratic form on a graph and show the characterization of eigenvalues and eigenvectors of the Laplacian in terms of this quadratic form.

Remember, an undirected graph $G = (V, E)$ is a set of vertices V and a set of connections, $E \subseteq V \times V$ between these vertices. We will assume that the graphs are unweighted and undirected until mentioned for the sake of simplicity. We will also assume that our graphs are simple unless otherwise stated.

In many cases we will be interested in regular graphs. A graph is d-regular if every vertex has degree d. Personally, I use n for the number of vertices and m for the number of edges. In case of regular graphs, mostly degree will be denoted by d.

Exercise 1. What is an upper bound on m? What is m for a d regular graph?

1 Matrices associated with graphs

Matrices provide a simple way to represent graphs. In general, most of the people represent graphs using a picture. This representation is not very useful as most of the information in the picture is useless (length and style of edges).

Assume that we are given labels of vertices (without loss of generality, we can assume that labels are number from 1 to n). Few concrete ways to represent a graph are,

- provide a list of edges,
- given a vertex, list all the neighbours,
- given a pair of vertices, output whether there is an edge or not.

Matrices provide a convenient representation for graphs. More importantly, graphs can be viewed as operators or a quadratic form using these representations. These operators give us a strong tool to analyse graph properties.

1.1 Adjacency matrix

The most common way to represent a graph is by its *adjacency matrix*. Given a graph G with n vertices, the adjacency matrix A_G of that graph is an $n \times n$ matrix whose rows and columns are labelled by the vertices. The (i, j)-th entry of the matrix A_G is 1 if there is an edge between vertices i and j and 0 otherwise.

Exercise 2. Show that the trace of an adjacency matrix is zero if the graph has no self loops.

Look at Fig. 1.1. What is its adjacency matrix? By definition, it should be a 6×6 matrix. Take a moment to write out the matrix and then check it with the result below.

$$\begin{pmatrix} 0&1&0&0&0&1 \\ 1&0&0&1&0&1 \\ 0&0&0&0&0&0 \\ 0&1&0&0&1&0 \\ 0&0&0&1&0&0 \\ 1&1&0&0&0&0 \end{pmatrix}$$

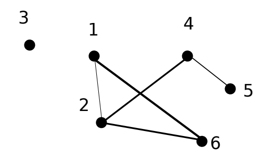

Fig. 1. Example of a cut with edges in the cut shown with solid line

Notice that the number of 1's in a row is equal to the degree of that vertex and A_G is a symmetric matrix. Suppose, graph G is regular. Then, every row of A_G has d ones.

Exercise 3. Show that A_G has an eigenvalue d.

You will show in the assignment that this is the biggest eigenvalue. From that proof, you can also see that the biggest eigenvalue is unique if the graph is connected.

Exercise 4. What can you say about the biggest eigenvalue of the adjacency matrix if the graph has 2 connected components?

1.2 Incidence matrix

We have already seen *incidence matrix* while discussing the linear program for min cut problem. For a graph, its incidence matrix is a rectangular matrix with rows indexed by edges and columns indexed by vertices. For the graph in Fig. 1.1, the incidence matrix will look like,

$$\begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{pmatrix}$$

The labelling of edges is not given. You can label the edges by looking at the incidence matrix given. Here, every row has 2 entries.

This matrix is not square and will not be useful in this course. If we assign a random direction to every edge and put 1 and -1 in every row instead of just 1, we will call it a directed incidence matrix.

1.3 Laplacian matrix

Say, D_G is a diagonal matrix of the graph G where the (i,i)-th entry has the degree of the i-th vertex. Then, the *Laplacian* of the graph is defined as,

$$L_G := D_G - A_G$$

Here, A_G is the adjacency matrix of the graph G. In other words, Laplacian matrix of a graph is the matrix which has degrees of the vertices in the diagonal, (i,j)-th entry is -1 if there is an edge and 0 otherwise.

Exercise 5. Let M_G be any directed incidence matrix of a graph, show,

$$L_G = M_G^T M_G.$$

Look at Fig. 1.1. What is its Laplacian matrix? By definition, it should be a 6×6 matrix. Take a moment to write out the matrix and then check it with the result below.

$$\begin{pmatrix} 2 & -1 & 0 & 0 & 0 & -1 \\ -1 & 3 & 0 & -1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & -1 & 1 & 0 \\ -1 & -1 & 0 & 0 & 0 & 2 \end{pmatrix}$$

In case of d-regular graphs, eigenvalues and eigenvectors of the Laplacian are deeply connected with those of the adjacency matrix. For a d-regular graph,

$$L_G = dI - A_G.$$

Exercise 6. Show that if u is an eigenvector of A_G with eigenvalue λ, then u is an eigenvector of L_G with eigenvalue $d - \lambda$.

From the discussion of the eigenvalues of A_G, we can infer that L_G is positive semidefinite for a d-regular graph. We will see in the next section that Laplacian is positive semidefinite for every graph.

An adjacency matrix encodes degrees in the graph only implicitly. So, Laplacian matrix will be used most of the time to represent a graph. In case of regular graphs, adjacency matrix and Laplacian are closely related; so, as a thumb rule, adjacency matrix is mostly useful when the graph is regular.

2 Quadratic form for the Laplacian

The Laplacian matrix lets us define a very important quadratic form for the graph,

$$x^T L_G x = \sum_{(i,j) \in E} (x_i - x_j)^2. \tag{1}$$

The proof of the above equation can be obtained by the definition of Laplacian and some calculation. We will give another proof in the inductive fashion.

Look at the simplest graph with two vertices and an edge between them. The Laplacian for this graph is,

$$L = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

If we label the vertices i and j, the quadratic form $x^T L x$ becomes,

$$x_i^2 - 2x_i x_j + x_j^2 = (x_i - x_j)^2.$$

If we have an n vertex graph, we can associate a Laplacian to every edge i, j,

$$L_{(i,j)}(e_i - e_j)(e_i - e_j)^T.$$

Here, e_i is the vector with i-th entry one and zero otherwise. The quadratic form $x^T L_{(i,j)} x$ becomes,

$$(x_i - x_j)^2.$$

Here, x_i is the i-th coordinate of x.

Exercise 7. Convince yourself that,

$$L_G = \sum_{(i,j)\in E} L_{(i,j)}.$$

Hence, we get the quadratic form, Eqn. 1, mentioned in the beginning of this section.

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

Since the quadratic form is sum of squares, it gives a direct proof that L_G is positive semidefinite.

Exercise 8. Show that for every graph G, there is an eigenvector of L_G with eigenvalue 0.

The only way this quadratic form can be zero is if $x_i = x_j$ whenever there is an edge (i,j). In other words, this quadratic form is zero iff $x_i = x_j$ for every i and j in the same connected component.

2.1 Eigenvalue characterization in terms of the quadratic form

The eigenvalues of a symmetric matrix can be characterized in terms of its quadratic form. For this section, assume that we have a symmetric matrix M and its eigenvalues are arranged in the ascending order,

$$\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n,$$

with eigenvectors $x_1, x_2, \cdots, x_n$.

Suppose, x is an eigenvector with eigenvalue λ. Then,

$$x^T M x = \lambda.$$

Since the quadratic form can be scaled arbitrarily by scaling the vector x, let us focus only on unit vectors.

If we look at all the eigenvectors of M, then the minimum quadratic form is obtained by the eigenvector of λ_1. Can the quadratic form be smaller than λ_1?

We know that $x_1, x_2, \cdots, x_n$ form an orthonormal basis by spectral decomposition. So, any unit vector $x \in \mathbb{R}^n$ can be written as,

$$x = \sum_i \alpha_i x_i,$$

with $\sum_i |\alpha_i|^2 = 1$.

Using spectral decomposition form of M,

$$x^T M x = \sum_i \alpha_i^2 \lambda_i.$$

Here, α_i^2 sum up to 1.

Exercise 9. Show that for every unit vector x,

$$x^T M x \geq \lambda_1.$$

This gives a characterization of the minimum eigenvalue λ_i,

$$\lambda_1 = \min_{x:\|x\|=1} x^T M x.$$

It is same as the equation,

$$\lambda_1 = \min_x \frac{x^T M x}{x^T x}.$$

Exercise 10. Why are the above two definitions of λ_1 same?

Using similar proof strategy, we can characterize other eigenvalues too.

$$\lambda_i = \min_{x:\|x\|=1,\ x\perp x_1,\cdots,x_{i-1}} x^T M x.$$

The proof is given as an assignment.

The characterization of λ_i can be made independent of eigenvectors.

Theorem 1 (Courant-Fischer). *Let M be a symmetric $n \times n$ matrix with eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$. Then,*

$$\lambda_k = \min_{S:dim(S)=k} \max_{x\in S:\|x\|=1} x^T M x.$$

Here, S is a subspace of $\mathbb{R}^n$. Also,

$$\lambda_k = \max_{S:dim(S)=n-k+1} \min_{x\in S:\|x\|=1} x^T M x.$$

Proof. The easy direction is to prove that there exist S, such that, λ_k is attained. S is precisely the space spanned by first k eigenvectors $x_1, x_2 \cdots, x_k$.

Exercise 11. Show that for the space S,

$$\max_{x\in S:\ \|x\|=1} x^T M x = \lambda_k.$$

For the opposite direction, we need to show that for every k dimensional S, there exists a unit vector $x \in S$ for which quadratic form is at least λ_k.

First, consider the space S' spanned by the last $n-k+1$ eigenvectors $x_k, x_{k+1}, \cdots, x_n$. By the arguments above, you can show that the quadratic form is greater than or equal to λ_k for every unit vector x in S'.

Exercise 12. Show that if S is a k dimensional subspace,

$$S \cap S' \neq \{0\}.$$

This completes the proof, because for every k-dimensional S, we have a unit vector whose quadratic form is at least λ_k (the one common with S'). The second part of the proof follows from a similar argument and given as an assignment. ☐

3 Assignment

Exercise 13. Calculate the eigenvectors and eigenvalues of the complete graph K_n.

Exercise 14. Show that for a d-regular graph, every eigenvalue of A_G is between d and $-d$.

Exercise 15. Show that the dimension of zero eigenspace of L_G is equal to the number of connected components in G.

Exercise 16. Show that the i-th eigenvalue of a symmetric matrix can be written as,

$$\lambda_i = \min_{x:\|x\|=1,\ x\perp x_1,\cdots,x_{i-1}} x^T M x,$$

where x_i's are the corresponding eigenvectors.

Exercise 17. Read about Perron-Frobenius theorem for symmetric entry-wise positive matrices. What are its implications for the adjacency matrix?

Exercise 18. Let M be a symmetric $n \times n$ matrix with eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$. Then show that,

$$\lambda_k = \min_{S:\ dim(S)=k} \max_{x\in S:\ \|x\|=1} x^T M x.$$