

CptS 591: Elements of Network Science, Spring 2021

Spectral Analysis, Part II

Lecture Notes

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In the last lecture (Spectral Analysis I), we reviewed some basic linear algebra concepts we need for spectral analysis. In these notes, we will see how the spectra of several different types of matrices associated with a graph can be used to analyze a graph.

References for these notes include: (1) Baltz and Kliemann, Spectral Analysis (Chapter 14 in Network Analysis (Brandes and Erlebach, Editors)) and (2) Dan Spielman's class on Spectral Graph Theory, Fall 2015.

1 Matrices for Graphs

We will in particular look at three matrices associated with graphs: the *adjacency* matrix, the *Laplacian*, and the *normalized Laplacian*. Let $G = (V, E)$ be the graph, and let $V = \{1, 2, \dots, n\}$.

1.1 Spectrum of the adjacency matrix

The adjacency matrix A_G is defined such that entry $A_G(u, v) = 1$ if $(u, v) \in E$ and 0 otherwise.

Let $w \in \mathbb{C}^n$ be an arbitrary vector and let $\omega : V \rightarrow \mathbb{C}$ map each $i \in V$ on w_i . Then, the i th component of $A_G w$, $\sum_{j=1}^n a_{ij} w_j$, can be written as $\sum_{j \in N(i)} \omega(j)$. Now the equation $A_G x = \lambda x$ has the following useful interpretation.

Remark 1 *Two points:*

- A_G has eigenvalue λ if and only if there exists a nonzero weight function $\omega : V \rightarrow \mathbb{C}$ such that for all $i \in V$, $\lambda \omega(i) = \sum_{j \in N(i)} \omega(j)$.
- The Spectral Theorem ensures that we can restrict ourselves to considering real-valued weight functions. Moreover, we can assume the maximum weight to be non-negative (if $\max\{\omega(i); i \in V\} < 0$ then $\omega(i) < 0$ for all $i \in V$ and we can consider $-\omega$ instead of ω).

Remark 1 enables us prove the following claims:

Lemma 1 Let $G = (V, E)$ be a graph on n vertices with adjacency matrix A_G and eigenvalues $\lambda_1 \leq \dots \leq \lambda_n$. Let Δ be the maximum vertex degree in G .

1. $\lambda_n \leq \Delta$.
2. If $G = G_1 \cup G_2$ is the union of two disjoint graphs G_1 and G_2 then $\text{spectrum}(A_G) = \text{spectrum}(A_{G_1}) \cup \text{spectrum}(A_{G_2})$.
3. If G is bipartite then $\lambda \in \text{spectrum}(G) \iff -\lambda \in \text{spectrum}(G)$.
4. If G is a simple cycle then $\text{spectrum}(G) = \{2 \cos(\frac{2\pi k}{n}); k \in \{1, \dots, n\}\}$.

Let us now see the spectra of the complete bipartite graph K_{n_1, n_2} and the complete graph K_n .

Lemma 2 Let n_1, n_2 and n be positive integers.

1. For $G = K_{n_1, n_2}$, $\lambda_1 = -\sqrt{n_1 n_2}, \lambda_2 = \dots = \lambda_{n-1} = 0$, and $\lambda_n = \sqrt{n_1 n_2}$.
2. For $G = K_n$, $\lambda_1 = \dots = \lambda_{n-1} = -1, \lambda_n = n - 1$.

The adjacency matrix is also useful for counting paths of length k in a graph.

Lemma 3 Let G be a multi-digraph possibly with loops. The (i, j) th entry of A^k counts the $i \rightarrow j$ -paths of length k . The eigenvalues of A^k are λ_i^k .

Corollary 1 The following hold true:

- $\sum_{i=1}^n \lambda_i = \text{number of loops in } G$.
- $\sum_{i=1}^n \lambda_i^2 = 2 \cdot |E|$.
- $\sum_{i=1}^n \lambda_i^3 = 6 \times \text{the number of triangles in } G$.

Using these we can prove the third claim in Lemma 1.

Lemma 4 G is bipartite if and only if the eigenvalues of A_G occur in pairs λ, λ' such that $\lambda = -\lambda'$.

Things the spectrum of the adjacency matrix does not help with Consider two graphs: a star graph on 5 vertices, and a five-vertices graph made up of a four-cycle and an isolated vertex. The two graphs have eigenvalues $\lambda_1 = -2, \lambda_2 = \lambda_3 = \lambda_4 = 0$ and $\lambda_5 = 2$, but they are not isomorphic. Such graphs are called *cospectral*. Also, we cannot determine from the spectrum of A_G whether or not G is connected. Fortunately, this can be addressed using the spectrum of the Laplacian, which we will see in the next section.

1.2 Spectrum of the Laplacian

Let D_G be the diagonal matrix in which $D(i, i)$ is the degree of vertex i , $d(i)$. The Laplacian matrix of the graph G is defined as $L_G = D_G - A_G$. If G is a simple, undirected graph, then, l_{ij} , the (i, j) th entry of L_G is

$$l_{i,j} = \begin{cases} -1 & \text{if } (i, j) \in E, \\ d(i) & \text{if } i = j, \\ 0 & \text{otherwise.} \end{cases} \quad (1)$$

There is also another way of defining the Laplacian matrix that provides some useful insights. This requires *orienting* (assigning direction) to the edges of G . Let σ be some orientation of G , that is, for every edge $e = (i, j)$ in G , σ specifies the head and the tail of the directed edge. The *incidence matrix* B_{G_σ} is a matrix whose rows are indexed by the vertices of G , whose columns are indexed by the edges of G , and each of its entries $b_{i,e}$ is such that

$$b_{i,e} = \begin{cases} 1 & \text{if } i \text{ is the head of } e, \\ -1 & \text{if } i \text{ is the tail of } e, \\ 0 & \text{otherwise.} \end{cases} \quad (2)$$

It can be shown that, independently of the choice of σ , $L_G = B_G B_G^T$. Consequently, we have the following result. First a word on notation: here and elsewhere, I will at times drop the subscript G to simplify notation.

Lemma 5 *For any vector $x \in \mathbb{C}^n$, $x^T L x = x^T B B^T x = \sum_{(i,j) \in E} (x_i - x_j)^2$.*

Lemma 5 has several important implications—we shall return to one of these a bit later in this lecture. Since the adjacency matrix A is real and symmetric, the Laplacian $L (= D - A)$ is also symmetric. Hence the Laplacian has n real eigenvalues $\lambda_1(L) \leq \lambda_2(L) \leq \dots \leq \lambda_n(L)$. As we have done in the case of the adjacency matrix in section 1.1, we may interpret an eigenvector $x \in \mathbb{R}^n$ as an assignment of weights $\omega : V \rightarrow \mathbb{R}$, $i \rightarrow x_i$. Then, λ is an eigenvalue of L if there exists a non-zero weight function $\omega \rightarrow \mathbb{R}$ such that

$$\lambda \omega(i) = \sum_{j \in N(i)} (\omega(i) - \omega(j)) \quad (3)$$

for all $i \in V$.

One of the good uses of the Laplacian is its relationship with connected components in a graph.

Lemma 6 *A graph G consists of k connected components if and only if $\lambda_1(L) = \dots = \lambda_k(L) = 0$ and $\lambda_{k+1}(L) > 0$.*

1.3 The normalized Laplacian

The spectrum of the Laplacian helps us count connected components, but it fails to tell us whether or not a graph is bipartite. We saw in section 1.1 that the spectrum of the adjacency matrix helps us determine whether or not a graph is bipartite, but that spectrum does not tell us anything about the graph's connected components. There is a matrix we can associate with a graph that helps us achieve both. It is called the *normalized Laplacian* and is defined as $\mathcal{L} = D^{-1/2} L D^{-1/2}$, where D , as defined earlier, is the diagonal matrix whose entry $D(i, i)$ is degree $d(i)$ and L is the Laplacian. For simple graphs, \mathcal{L} satisfies

$$\mathcal{L}(i, j) = \begin{cases} 1 & \text{if } i = j \text{ and } d(i) > 0, \\ -\frac{1}{\sqrt{d(i)d(j)}} & \text{if } (i, j) \in E, \\ 0 & \text{otherwise.} \end{cases} \quad (4)$$

Like the Laplacian, \mathcal{L} is also symmetric, and its eigenvalues are real and they can be ordered as $\lambda_1(\mathcal{L}) \leq \dots \leq \lambda_n(\mathcal{L})$. Moreover, using similar arguments as in the other two cases we saw, λ is an eigenvalue of \mathcal{L} if there is a non-zero weight function $\omega : V \rightarrow \mathbb{C}$, such that

$$\lambda\omega(i) = \frac{1}{\sqrt{d(i)}} \sum_{j \in N(i)} \left(\frac{\omega(i)}{\sqrt{d(i)}} - \frac{\omega(j)}{\sqrt{d(j)}} \right). \quad (5)$$

Among many others, we can state the following results on the spectrum of \mathcal{L} .

Lemma 7 *Let G be a graph and \mathcal{L} be its normalized Laplacian matrix. The following hold:*

1. $\lambda_1(\mathcal{L}) = 0$, $\lambda_n(\mathcal{L}) \leq 2$.
2. G is bipartite if and only if for each $\lambda(\mathcal{L})$, the value $2 - \lambda(\mathcal{L})$ is also an eigenvalue of \mathcal{L} .
3. If $\lambda_1(\mathcal{L}) = \dots = \lambda_k(\mathcal{L}) = 0$ and $\lambda_{k+1} \neq 0$, then G has exactly k connected components.

2 The second-smallest eigenvalue of the Laplacian

In Lemma 5, we saw that, for any vector x associated with the vertices of a graph, the Laplacian L of the graph satisfies $x^T Lx = \sum_{(i,j) \in E} (x_i - x_j)^2$ (the Laplacian quadratic form). As all of the terms in the sum are squares, we can see that the quadratic form is never negative. If we let x be a constant vector, then the form is zero. So, the smallest eigenvalue of the Laplacian is zero. If the graph is connected, then, by Lemma 6, the second-smallest eigenvalue $\lambda_2(L) > 0$. The magnitude of $\lambda_2(L)$ reflects how well connected the graph is. For this reason, Miroslav Fiedler, the mathematician who first developed the theory around this, called λ_2 the “algebraic connectivity of a graph”. In his honor, the eigenvector associated with λ_2 is called the Fiedler vector.

Recall from the previous lecture the notion of the Rayleigh quotient of a vector x with respect to a matrix M : $x^T Mx / x^T x$. We saw that a vector x that *maximizes* this quotient is an eigenvector of M with eigenvalue equal to the quotient, and that the eigenvalue is the *largest*. A similar statement can be made about a vector that *minimizes* the quotient: the vector is an eigenvector, and the quotient is equal to the smallest (nonzero) eigenvalue. In summary, we have:

Lemma 8 *Given the Laplacian L .*

- *The largest eigenvalue λ_n satisfies:*

$$\lambda_n = \max_{x \in \mathbb{R}^n, x \neq 0_n} \frac{x^T Lx}{x^T x}$$

- *The second smallest eigenvalue λ_2 satisfies:*

$$\lambda_2 = \min_{x \perp 1_n} \frac{x^T Lx}{x^T x}$$

2.1 Isoperimetry

The second-smallest eigenvalue of the Laplacian λ_2 is also intimately related to the problem of dividing a graph into two pieces without cutting too many edges.

Let $S \subset V$ be subset of the vertices a graph $G = (V, E)$. One way of measuring how well S can be separated from the graph is to count the number of edges connecting S to the rest of the graph. These edges are called the *boundary* of S , and are defined as follows

$$\partial(S) = \{(u, v) \in E : u \in S, v \notin S\}.$$

The ratio of the number of boundary edges to the size of S is called the *isoperimetric ratio* of S and is defined as:

$$\theta(S) = \frac{|\partial(S)|}{|S|}.$$

The *isoperimetric number* of a graph is the minimum isoperimetric number over all sets of at most half the vertices:

$$\theta_G = \min_{|S| \leq n/2} \theta(S).$$

The following result states a lower bound on θ_G in terms λ_2 .

Theorem 1 For every $S \subset V$,

$$\theta(S) \geq \lambda_2(1 - s),$$

where $s = |S|/|V|$.

3 Spectra of subgraphs and super-graphs

Can the spectrum of a graph tell us anything about spectra of its subgraphs? Can the spectra of two graphs tell us anything about the spectrum of a larger graph derived by combining the two? We will see a couple of results (on spectrum of the adjacency matrix) that help answer such questions.

The first result is on induced subgraphs (it is called the Interlacing Theorem).

Theorem 2 Let $G = (V, E)$ be a graph on n vertices. Let H be an induced subgraph of G on m vertices. Let $\lambda_1 \leq \dots \leq \lambda_n$ be the eigenvalues of the adjacency matrix of G . Let $\mu_1 \leq \dots \leq \mu_m$ be the eigenvalues of the adjacency matrix of H . Then,

$$\lambda_i \leq \mu_i \leq \lambda_{i+(n-m)} \quad \forall i \in \{1, \dots, m\}.$$

In the simplest case of this, let H be the graph obtained from G by removing just one vertex. Then, the theorem tells us that between two eigenvalues of G there lies exactly one eigenvalue of H . Consequently, if G has an eigenvalue with multiplicity k , then H has this eigenvalue with multiplicity $k - 1$.

Our next results are about graphs obtained by combining other graphs. Consider two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$.

The *sum* $G_1 + G_2$ is a graph on $V_1 \times V_2$ where two vertices $(i_1, i_2), (j_1, j_2) \in V_1 \times V_2$ are connected if either (but not both) $(i_1, j_1) \in E_1$ or $(i_2, j_2) \in E_2$.

The *cartesian product* $G_1 \times G_2$ is a graph on $V_1 \times V_2$ where two vertices $(i_1, i_2), (j_1, j_2) \in V_1 \times V_2$ are connected if and only if $(i_1, j_1) \in E_1$ and $(i_2, j_2) \in E_2$.

We can state the following on the spectrum of the adjacency matrices.

Lemma 9 $\text{spectrum}(G_1 + G_2) = \text{spectrum}(G_1) + \text{spectrum}(G_2)$.
 $\text{spectrum}(G_1 \times G_2) = \text{spectrum}(G_1) \times \text{spectrum}(G_2)$.