MA431 Spectral Graph Theory: Lecture 1

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1 The spectrum of a graph

In this course, we shall work with graphs, matrices associated with them, and spectral features of those matrices. We shall see how these spectral aspects help in studying graphs, whether it be algebraic, algorithmic, or structural.

1.1 The adjacency matrix

Throughout this course, unless stated otherwise, graphs have no loops but may have parallel edges. For the most part, we will be working with graphs, but sometimes, it will be convenient to work in the more general framework of directed graphs. Like graphs, directed graphs have no loops but may have parallel or opposite arcs.

Definition 1.1. Let D be a directed graph. The *adjacency matrix* of D, denoted $A(D)$, is the square matrix whose rows and columns are indexed by the vertices (in the same order), where the uv-entry is equal to the number of arcs from u to v.

As D has no loops, the diagonal entries of $A(D)$ are equal to 0.

We may also define the adjacency matrix of a graph, by treating it as a directed graph where we have two opposite arcs with the same ends replacing every edge:

Definition 1.2. Let G be a graph. The *adjacency matrix* of G, denoted $A(G)$, is the square matrix whose rows and columns are indexed by the vertices, where the uv-entry is equal to the number of edges between u and v.

Observe that $A(G)$ is a real symmetric matrix whose diagonal entries are equal to 0.

1.2 The spectrum

Recall further that the spectrum of a real symmetric matrix is the list of its eigenvalues, where each eigenvalue with multiplicity k appears k times in the list; if the matrix is $n \times n$, then its spectrum has length n.

Definition 1.3. The *spectrum* of a graph G is the spectrum of its adjacency matrix $A(G)$. If G has n vertices, then its spectrum is denoted $\theta_1(G) \geq \cdots \geq \theta_n(G)$.

The eigenvectors of the adjacency matrix of a graph have a nice interpretation in terms of the graph itself:

Definition 1.4. The *eigenvectors* of a graph G are the eigenvectors of its adjacency matrix $A(G)$. Equivalently, a nonzero vector $f \in \mathbb{R}^{V(G)}$ is an *eigenvector* of G if for some $\theta \in \mathbb{R}$,

$$\theta \cdot f_v = \sum (f_u : \{u, v\} \text{ is an edge}) \qquad \forall v \in V(G).$$

(Note that f_u above is counted as many times as the number of edges between u, v.) The eigenvector f is *associated* with the eigenvalue θ.

As an immediate consequence,

Corollary 1.5. Given a d-regular graph, the all-ones vector is an eigenvector with corresponding eigenvalue d.

Let A be an $n \times n$ real symmetric matrix. Recall that the characteristic polynomial of A is $p_A(x) := \det(xI - A)$, where I is the $n \times n$ identity matrix. Equivalently, if $\theta_1, \ldots, \theta_n$ denotes the spectrum of A, then $p_A(x) = \Pi_{i=1}^n (x - \theta_i)$.

Definition 1.6. The *characteristic polynomial* of a graph G is the characteristic polynomial of its adjacency matrix $A(G)$.

1.3 Counting directed walks

Let D be a directed graph. A *directed walk of length ℓ* is a sequence of vertices $(v_0, v_1, \ldots, v_\ell)$, where for each $i \in [\ell] := \{1, \ldots, \ell\}$, there is an arc from v_{i-1} to v_i. Note that some of the vertices in the sequence may be equal. In particular, if $v_0 = v_\ell$, then the directed walk is *closed*.

Proposition 1.7. Let D be a directed graph, let $A := A(D)$, and take an integer $\ell \geq 1$. Then for all possibly equal vertices u and v, the number of directed walks from u to v of length ℓ is equal to $(A^\ell)_{uv}$. In particular, $\mathrm{tr}(A^\ell)$ is equal to the number of closed directed walks of length ℓ.

Proof. Exercise. □

Subsequently,

Proposition 1.8. Let G be a simple graph with m edges and t triangles, and let $A := A(G)$.[1] Then $\mathrm{tr}(A) = 0$, $\mathrm{tr}(A^2) = 2m$, and $\mathrm{tr}(A^3) = 6t$.

Proof. Exercise. □

Recall that the trace of a real symmetric matrix, being the sum of its diagonal entries, is equal to the sum of the eigenvalues in its spectrum. Recall further that the eigenvalues of A^ℓ are the ℓ^{th} powers of the eigenvalues of A. Combined with the preceding proposition, we can conclude that the spectrum of a simple graph determines its number of vertices, edges, and triangles:

Corollary 1.9. Let G be an n-vertex simple graph with m edges, and t triangles, whose spectrum is $\theta_1, \ldots, \theta_n$. Then $\sum_{i=1}^n \theta_i = 0$, $\sum_{i=1}^n \theta_i^2 = 2m$ and $\sum_{i=1}^n \theta_i^3 = 6t$.

[1] Recall that a graph is simple if it has no loops or parallel edges.

1.4 Cospectral graphs

Two graphs are *cospectral* if they have the same spectrum, i.e. the same eigenvalues with the same multiplicities. One important example comes from isomorphic pairs:

Proposition 1.10. Let D, D' be isomorphic directed graphs. Then the following statements hold:

1. $A(D)$ and $A(D')$ are similar matrices.

2. $p_{A(D)}(x) = p_{A(D')}(x)$.

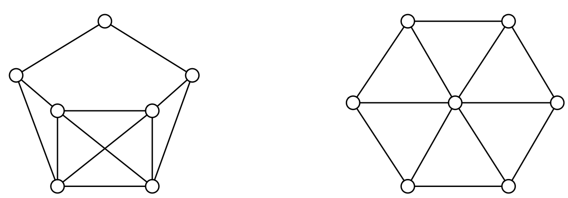
3. $A(D), A(D')$ have the same eigenvalues with the same algebraic and geometric multiplicities.

Consequently, isomorphic graphs are cospectral.

Proof. **(1)** Let $A := A(D)$ and $A' := A(D')$. Since D, D' are isomorphic, there exists a permutation matrix P such that $A' = P^\top AP$. Since $P^\top = P^{-1}$, it follows that A' and A are similar. **(2)** and **(3)** follow from (1) by using Basic Linear Algebra. □

There are other examples of cospectral pairs; that is, the spectrum does not determine the isomorphism class of a graph. For example, the two graphs $K_{1,4}, K_1 \cup C_4$, defined in §1.5 for clarity, share the spectrum $2, 0, 0, 0, -2$, so they are cospectral, even though they are clearly not isomorphic. (There are also cospectral graphs with the same degree sequence that are non-isomorphic. See Figure 1 and Problem 13.)

A planar graph may even be cospectral to a non-planar graph; that is, the spectrum does not determine planarity either. For example, the two graphs shown below share the spectrum $-2, 1-\sqrt{7}, -1, -1, 1, 1, 1+\sqrt{7}$.



1.5 Examples

Example 1.11. Consider the graph $K_{1,4}$ with vertices $\{1, 2, 3, 4, 5\}$ and edges $\{1, 2\}, \{1, 3\}, \{1, 4\}, \{1, 5\}$. This graph has the following spectrum:

- -2: the corresponding eigenspace is generated by $(-2, 1, 1, 1, 1)^\top$,

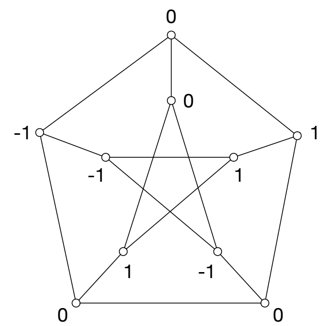
- $0^{(3)}$: the corresponding eigenspace is generated by $(0, 1, -1, 0, 0)^\top$, $(0, 1, 1, -2, 0)^\top$ and $(0, 1, 1, 1, -3)^\top$,

- 2: the corresponding eigenspace is generated by $(2, 1, 1, 1, 1)^\top$.

Example 1.12. Consider the graph $K_1 \cup C_4$ with vertices $\{1, 2, 3, 4, 5\}$ and edges $\{2, 3\}, \{3, 4\}, \{4, 5\}, \{5, 2\}$. This graph has the following spectrum:

- -2: the corresponding eigenspace is generated by $(0,1,-1,1,-1)^\top$,
- $0^{(3)}$: the corresponding eigenspace is generated by $(1,0,0,0,0)^\top$, $(0,1,0,-1,0)^\top$ and $(0,0,1,0,-1)^\top$,
- 2: the corresponding eigenspace is generated by $(0,1,1,1,1)^\top$.

Example 1.13. An eigenvector of the Petersen graph with eigenvalue 1 is shown below:



2 The Perron-Frobenius Theorem

Let A be an $n \times n$ real symmetric matrix, and let $\theta \in \mathbb{R}$. A vector $x \in \mathbb{R}^n$ is θ-*subharmonic* if $x \geq \mathbf{0}$, $x \neq \mathbf{0}$, and $Ax \geq \theta x$. In the remark below, we see how eigenvectors naturally lead to subharmonic vectors. Note that $|A|$ refers to the matrix obtained from A after replacing each entry by its absolute value, and $|x|$ is defined similarly.

Remark 2.1. Let A be a real symmetric matrix, and let x be an eigenvector with eigenvalue θ. Then $|x|$ is $|\theta|$-subharmonic for the matrix $|A|$. In particular, if A is nonnegative, then $|x|$ is $|\theta|$-subharmonic for the matrix A.

Proof. We have $|A||x| \geq |Ax| = |\theta x| = |\theta||x|$, where the first inequality follows from the fact that $|\cdot|$ is a metric and therefore satisfies the triangle inequality. Thus, $|x|$ is $|\theta|$-subharmonic for $|A|$. □

Let A be an $n \times n$ real symmetric matrix. The *underlying graph of* A is the on n vertices corresponding to the common labels of the rows and columns of A, where an edge between u, v exists if and only if $A_{uv} \neq 0$. Observe that this graph *may* have loops. We say that A is *irreducible* if this graph is connected.

Lemma 2.2. Let A be a real symmetric matrix that is nonnegative and irreducible. Then there exists a maximum real number ρ such that there is a ρ-subharmonic vector for A. Moreover, every ρ-subharmonic vector x is an eigenvector with eigenvalue ρ, and satisfies $x > \mathbf{0}$. In particular, ρ is an eigenvalue.

Proof. Let $\rho := \max\left\{x^\top Ax : x^\top x = 1\right\}$. By the Courant-Fischer Theorem, ρ is the largest eigenvalue of the matrix A, and the maximum is achieved only by vectors in the ρ-eigenspace. We claim that this is the desired ρ.

First, we need to prove that there is a ρ-subharmonic vector. Since $\operatorname{tr}(A) \geq 0$, it follows that $\rho \geq 0$. Thus, the previous lemma implies that there is a ρ-subharmonic vector.

Secondly, we need to prove that there is no ρ'-subharmonic vector x', for any $\rho' > \rho$. Suppose otherwise. After a normalisation, if necessary, we may assume that $x'^{\top}x' = 1$ (recall $x' \neq \mathbf{0}$). Then $x'^{\top}Ax' \geq x'^{\top}(\rho' x') = \rho'$ (recall $x' \geq \mathbf{0}$). But our choice of ρ implies that $x'^{\top}Ax' \leq \rho$, a contradiction.

Thirdly, pick a ρ-subharmonic vector x. We need to prove that x lies in the eigenspace of ρ. After a normalisation, if necessary, we may assume that $x^{\top}x = 1$. Then

$$\rho \geq x^{\top}Ax \geq x^{\top}(\rho x) = \rho,$$

where the first inequality follows from the maximal choice of ρ, and the second one from the choice of x. Thus, equality must hold throughout, so $x^{\top}Ax = \rho$, so x must lie in the eigenspace of ρ.

Finally, it remains to show that $x > \mathbf{0}$. Suppose otherwise. The irreducibility of A implies the existence of indices u, v such that $x_u = 0, x_v > 0$ and $(A)_{uv} > 0$. But then

$$0 = (\rho x)_u = (Ax)_u = \sum_w (A)_{uw}x_w \geq (A)_{uv}x_v > 0,$$

a contradiction. $\square$