Lecture 12. Eigenvalues of graphs

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Hermitian matrices

Goal. Give an introduction to the study of graphs via their eigenvalues. This will involve some linear algebra.

We begin with the review of some linear algebra. We will be interested in properties of eigenvalues of symmetric real matrices. A more natural framework: Hermitian complex matrices.

Definition. A square complex matrix $A = (a_{ij}) \in M_n(\mathbf{C})$ is Hermitian if $A^{\mathrm{t}} = \overline{A}$; explicitly, we have

$$a_{ji} = \overline{a_{ij}} \quad \text{for all} \quad 1 \leq i, j \leq n.$$

Note: if $A \in M_n(\mathbf{R})$, then $\overline{A} = A$, hence A is Hermitian if and only if it is symmetric.

Hermitian matrices, cont'd

Recall that $\mathbf{C}^n$ carries a standard inner product $\langle -, - \rangle$ given by

$$\langle u, v \rangle = \sum_{i=1}^{n} u_i \overline{v_i} \quad \text{for} \quad u = (u_1, \ldots, u_n), v = (v_1, \ldots, v_n).$$

Key property: for all u, we have $\langle u, u \rangle \geq 0$, with equality if and only if $u = 0$.

If $A = (a_{ij})_{1 \leq i,j \leq n}$ is a matrix and $u = (u_1, \ldots, u_n) \in \mathbf{C}^n$, then A gives a linear map $A \colon \mathbf{C}^n \to \mathbf{C}^n$ such that $Au = (\sum_{i=1}^{n} a_{i,j} u_j)_{1 \leq i \leq n}$. It follows that if $u = (u_1, \ldots, u_n)$ and $v = (v_1, \ldots, v_n)$, then

$$\langle Au, v \rangle = \sum_{i,j=1}^{n} a_{ij} u_j \overline{v_i}.$$

If A is Hermitian, then it follows from the definition and the above formula that $\langle Au, v \rangle = \overline{\langle Av, u \rangle}$. In particular, we have $\langle Au, u \rangle \in \mathbf{R}$ for all u.

Hermitian matrices, cont'd

Recall: every $A \in M_n(\mathbf{C})$ has an eigenvalue λ; this means that there is $u \in \mathbf{C}^n$ nonzero (an eigenvector of λ) such that $Au = \lambda u$.
If A is Hermitian, we see $\langle Au, u\rangle = \langle \lambda u, u\rangle = \lambda \cdot \langle u, u\rangle$ is a real number. Since $\langle u, u\rangle$ is a positive real number, it follows $\lambda \in \mathbf{R}$. Hence all eigenvalues of A are real.

Starting with an eigenvector u for the Hermitian matrix A and taking $W = u^\perp := \{v \in \mathbf{C}^n | \langle u, v\rangle = 0\}$, we have $A(W) \subseteq W$: if $\langle u, w\rangle = 0$, then

$$\langle Aw, u\rangle = \overline{\langle Au, w\rangle} = \overline{\lambda} \cdot \overline{\langle u, w\rangle} = 0.$$

One can also see: with respect to an orthonormal basis of W, the restriction of A to W is given again by a Hermitian matrix, and we can iterate the discussion. One proves in this way: $\mathbf{C}^n$ has an orthonormal basis given by eigenvectors of A. In particular: A is diagonalizable.

The Min-Max Theorem

Let $A \in M_n(\mathbf{C})$ be a Hermitian matrix, with eigenvalues $\lambda_1 \leq \ldots \leq \lambda_n$. We consider the Rayleigh quotient

$$R_A(u) := \frac{\langle Au, u\rangle}{\langle u, u\rangle} \in \mathbf{R} \quad \text{for} \quad u \in \mathbf{C}^n \setminus \{0\}.$$

Clear: $R_A(u) = R_A(\alpha u)$ for all $\alpha \in \mathbf{C}$, $\alpha \neq 0$.
Theorem 1. For every k, with $1 \leq k \leq n$, we have

$$\lambda_k = \min\left\{ \max\{R_A(u) \mid u \in U, u \neq 0\} \mid U \subseteq \mathbf{C}^n, \dim(U) = k\right\}$$

$$= \max\left\{ \min\{R_A(u) \mid u \in V, u \neq 0\} \mid V \subseteq \mathbf{C}^n, \dim(V) = n-k+1\right\}.$$

In particular, we have $\lambda_n = \max\left\{R_A(u) \mid u \in \mathbf{C}^n \setminus \{0\}\right\}$ and $\lambda_1 = \min\left\{R_A(u) \mid u \in \mathbf{C}^n \setminus \{0\}\right\}$.

Proof of the Min-Max Theorem

Let's start with the first equality. We have seen that we can choose an orthonormal basis $u_1, \ldots, u_n$ of $\mathbf{C}^n$ consisting of eigenvectors of A corresponding to $\lambda_1, \ldots, \lambda_n$.

If $U \subseteq \mathbf{C}^n$ has dimension k, then

$$U \cap \mathrm{LinearSpan}(u_k, \ldots, u_n) \neq \{0\}.$$

If $0 \neq u = \sum_{i=k}^n \alpha_i u_i$ lies in this intersection, then

$$R_A(u) = \frac{\langle \sum_{i=k}^n \lambda_i \alpha_i u_i, \sum_{i=k}^n \alpha_i u_i \rangle}{\langle \sum_{i=k}^n \alpha_i u_i, \sum_{i=k}^n \alpha_i u_i \rangle} = \frac{\sum_{i=k}^n \lambda_i \cdot |\alpha_i|^2}{\sum_{i=k}^n |\alpha_i|^2} \geq \lambda_k.$$

Hence $\lambda_k \leq \min \left\{ \max\{R_A(u) \mid u \in U, u \neq 0\} \mid U \subseteq \mathbf{C}^n, \dim(U) = k \right\}$.

Proof of the Min-Max Theorem, cont'd

For the reverse inequality, we need to find a subspace U of $\mathbf{C}^n$ of dimension k such that

$$\lambda_k \geq \max\{R_A(u) \mid u \in U, u \neq 0\}.$$

We take $U = \mathrm{LinearSpan}(u_1, \ldots, u_k)$. If $u = \sum_{i=1}^k \alpha_i u_i \in U$ is nonzero, then

$$R_A(u) = \frac{\langle \sum_{i=1}^k \lambda_i \alpha_i u_i, \sum_{i=1}^k \alpha_i u_i \rangle}{\langle \sum_{i=1}^k \alpha_i u_i, \sum_{i=1}^k \alpha_i u_i \rangle} = \frac{\sum_{i=1}^k \lambda_i \cdot |\alpha_i|^2}{\sum_{i=1}^k |\alpha_i|^2} \leq \lambda_k.$$

This completes the proof of the first assertion.

Proof of the Min-Max Theorem, cont'd

Note now that $-A$ is again Hermitian and $R_{-A}(u) = -R_A(u)$ for all $u \neq 0$. Moreover, if $\lambda'_1 \leq \ldots \leq \lambda'_n$ are the eigenvalues of $-A$, then it is clear that $\lambda'_i = -\lambda_{n+1-i}$. If we apply the first assertion in the theorem for $-A$, we obtain the second assertion. This completes the proof of the theorem.

Suppose that A is a Hermitian $n \times n$ matrix as before and $\lambda_1 \leq \ldots \leq \lambda_n$ are the eigenvalues of A. We have seen that if $\mathbf{C}^n \ni u \neq 0$, then $R_A(u) \leq \lambda_n$. We will make use of the following

Exercise. Show that if $u \in \mathbf{C}^n$ is nonzero, then $R_A(u) = \lambda_n$ if and only if u is an eigenvector of A corresponding to λ_n.

Interlacing

With A as before, consider an $m \times m$ submatrix B of A, obtained by deleting rows and columns with the same indices. Note that in this case B is Hermitian, too, and say its eigenvalues are $\mu_1 \leq \ldots \leq \mu_m$.

Corollary (Interlacing). With the above notation, we have

$$\lambda_j \leq \mu_j \leq \lambda_{j+n-m} \quad \text{for} \quad 1 \leq j \leq m.$$

Proof. Consider the linear subspace $W \simeq \mathbf{C}^m$ generated by the standard basis vectors of $\mathbf{C}^n$ corresponding to the indices of the rows/columns in B. Then B gives a linear map $W \to W$ such that for every $u \in W$, we have

$$A(u) = B(u) + w \quad \text{for some} \quad w \in W^{\perp}.$$

Then $\langle Au, u \rangle = \langle Bu, u \rangle$, hence $R_A(u) = R_B(u)$ for every $u \in W$.
We get $\lambda_j \leq \mu_j$ by 1st formula in Min-Max Theorem and $\mu_j \leq \lambda_{j+n-m}$ by the 2nd formula in Min-Max Theorem.

Eigenvalues for graphs

Let G be a finite simple graph. Let's label its vertices as $1, 2, \ldots, n$.

Recall that the adjacency matrix is the matrix $A_G = (a_{ij}) \in M_n(\mathbf{R})$, where $a_{ij} = 1$ if i and j are adjacent and $a_{ij} = 0$ otherwise (in particular, we have $a_{ii} = 0$ for all i).
Remark. The matrix A_G is a symmetric real matrix, with non-negative entries.

The Laplacian of G is the matrix $L_G = (L_{ij}) \in M_n(\mathbf{R})$, where $L_{ii} = \deg(i)$ for $1 \leq i \leq n$ and $L_{ij} = -a_{ij}$ for $i \neq j$.
Example. If G is d-regular, then $L_G = dI_n - A_G$.
Remark. The matrix L_G is a symmetric real matrix.

Since A_G and L_G are symmetric real matrices, they have real eigenvalues. We order them as $\mu_1 \geq \ldots \geq \mu_n$ for A_G and $\lambda_1 \leq \ldots \leq \lambda_n$ for L_G.

Eigenvalues for graphs, cont'd

Remark. The reason for the reverse ordering of the eigenvalues: if G is d-regular, then $L = dI_n - A_G$, hence

$$\det(xI_n - L_G) = \det\big((x-d)I_n + A_G\big) = (-1)^n \cdot \det\big((d-x)I_n - A_G\big),$$

hence $\lambda_i = d - \mu_i$ for $1 \leq i \leq n$.

Remark. Since $\mathrm{trace}(A_G) = 0$, we have $\mu_1 + \ldots + \mu_n = 0$. We thus have $\mu_1 > 0$ and $\mu_n < 0$, unless $\mu_1 = \ldots = \mu_n = 0$, which can only happen if $E(G) = \emptyset$ (note that since A_G is symmetric, it is diagonalizable, and thus all eigenvalues are 0 if and only if $A_G = 0$.

Remark. The eigenvalues of A_G and L_G are independent of how we order the vertices: reordering the vertices corresponds to permuting the rows and columns of these matrices by the same permutation.

Eigenvalues for graphs, cont'd

Remark. If $A_G = (a_{ij})$ and $d_i = \deg(i)$, then for every $u = (u_1, \ldots, u_n) \in \mathbf{R}^n$, we have

$$\langle L_G u, u \rangle = \sum_{i=1}^{n} d_i u_i^2 - \sum_{i,j=1}^{n} a_{ij} u_i u_j = \sum_{i=1}^{n} d_i u_i^2 - 2 \sum_{ij \in E(G)} u_i u_j$$

$$= \sum_{ij \in E(G)} (u_i - u_j)^2.$$

Hence $\langle L_G(u), u \rangle \geq 0$ for every u (that is, L_G is semipositive), with equality if and only if $u_i = u_j$ whenever i and j lie in the same connected component of G. This implies that $\lambda_i \geq 0$ for all i.

Note also: $L_G(1, \ldots, 1) = \sum_{i=1}^{n} d_i - 2 \sum_{ij \in E(G)} 1 = 0$, hence 0 is an eigenvalue of L_G. We conclude that $\lambda_1 = 0$.

Example 1: complete graphs

Let us consider the complete graph K_n on n vertices, so that A_{K_n} is the $n \times n$ matrix

$$\begin{bmatrix} 0 & 1 & 1 & \dots & 1 \\ 1 & 0 & 1 & \dots & 1 \\ \dots & \dots & \dots & \dots & \dots \\ 1 & 1 & 1 & \dots & 0 \end{bmatrix}$$

Let $D_n := \det(xI_n - A_G) =$

$$\det \begin{bmatrix} x & -1 & -1 & \dots & -1 \\ -1 & x & -1 & \dots & -1 \\ -1 & -1 & x & \dots & -1 \\ \dots & \dots & \dots & \dots & \dots \\ -1 & -1 & -1 & \dots & x \end{bmatrix} = \det \begin{bmatrix} x & -1 & -1 & \dots & -1 \\ -x-1 & x+1 & 0 & \dots & 0 \\ -x-1 & 0 & x+1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ -x-1 & 0 & 0 & \dots & x+1 \end{bmatrix}$$

Expanding along the last row, we get $D_n = (x+1)D_{n-1} + (-1)^{n+1}(-x-1)(x+1)^{n-2}(-1)^{n+1} = (x+1)D_{n-1} - (x+1)^{n-1}$.

Example 1: complete graphs, cont'd

Since $D_1 = x$ and we have seen that

$$D_n = (x+1)D_{n-1} - (x+1)^{n-1} \quad \text{for} \quad n \geq 2,$$

it follows easily by induction that $D_n = (x+1)^{n-1}\big(x - (n-1)\big)$ (exercise: check this!).

Hence the eigenvalues of A_{K_n} are $\mu_1 = n-1$ and $\mu_2 = \ldots = \mu_n = -1$.

Since K_n is $(n-1)$-regular, it follows that the eigenvalues of L_{K_n} are $\lambda_1 = 0$ and $\lambda_2 = \ldots = \lambda_n = n$.

Example 2: complete bipartite graphs

Let $K_{m,n}$ be the complete bipartite graph on two sets with m and n elements. After suitably ordering the vertices, we have

$$A = A_{K_{m,n}} = \begin{bmatrix} \mathbf{0}_{m,m} & \mathbf{1}_{m,n} \\ \mathbf{1}_{n,m} & \mathbf{0}_{n,n} \end{bmatrix},$$

where we denote by $\mathbf{a}_{p,q}$ the $p \times q$ matrix with all entries equal to a. It is clear that $\mathrm{rank}(A) = 2$. A is diagonalisable, hence precisely $m + n - 2$ of the eigenvalues of $A_{K_{m,n}}$ are equal to 0. Since $\mathrm{Trace}(A) = 0$, it follows that the eigenvalues of A are given by

$$\mu_1 = \lambda,\ \mu_2 = \ldots = \mu_{m+n-1} = 0,\ \mu_{m+n} = -\lambda,$$

for some $\lambda > 0$. To find λ, let us try to find an eigenvector $u \in \mathbf{R}^{m+n}$ of A, such that $u_i = a$ for $1 \leq i \leq m$ and $u_i = b$ for $m+1 \leq i \leq m+n$. Then $Au = \lambda u$ is equivalent to $nb = \lambda a$ and $ma = \lambda b$. Divide the second by the first to get $(b/a)^2 = m/n$, hence $\lambda = ma/b = m\sqrt{n/m} = \sqrt{mn}$.

The largest eigenvalue of A_G

Theorem 2. If G is a connected graph with n vertices and $\mu_1 \geq \ldots \geq \mu_n$ are the eigenvalues of A_G, then the following hold:

i) $\mu_1 \geq |\mu_k|$ for all k.

ii) The multiplicity of μ_1 is 1, that is, $\mu_1 > \mu_2$.

iii) There is an eigenvector $u = (u_1, \ldots, u_n)$ with eigenvalue μ_1 with $u_i > 0$ for all i.

The above result can be deduced from the Perron-Frobenius theorem concerning matrices with nonnegative entries. We will give a direct proof in our simpler case when the matrix is also symmetric.

We first give a general result about nonnegative eigenvectors for the adjacency matrix.

The largest eigenvalue of A_G, cont'd

Lemma. If G is a connected graph and $u = (u_1, \ldots, u_n)$ is an eigenvector for A_G with $u_i \geq 0$ for all i, then $u_i > 0$ for all i.

Proof. If λ is the eigenvalue corresponding to u, it follows that

$$\sum_{k=1}^{n} a_{ik} u_k = \lambda u_i \quad \text{for all} \quad 1 \leq i \leq n.$$

If $u_i = 0$ for some i, since $a_{ik} \geq 0$ and $u_k \geq 0$ for all k, we deduce that $a_{ik} u_k = 0$ for all k.

We thus see that if $u_i = 0$, then $u_j = 0$ for every neighbor j of i. Since G is connected, we easily deduce that $u_j = 0$ for all j, by induction on the length of the shortest path from i to j. We thus get $u = 0$, a contradiction.

The largest eigenvalue of A_G, cont'd

Proof of Theorem 2. The assertions are clear if $n = 1$, hence we may assume $n \geq 2$. We first show iii), namely that there is an eigenvector corresponding to μ_1 with positive entries. Let $v = (v_1, \ldots, v_n) \in \mathbf{R}^n$ be an eigenvector corresponding to μ_1 and let $u = (u_1, \ldots, u_n)$, with $u_i = |v_i|$ for all i. We then have

$$\mu_1 \cdot \langle v, v \rangle = |\langle A_G v, v \rangle| = \left| \sum_{i,j} a_{ij} v_i v_j \right| \leq \sum_{i,j} a_{ij} u_i u_j = \langle A_G u, u \rangle \leq \mu_1 \cdot \langle u, u \rangle,$$

where the last inequality follows from Theorem 1. On the other hand, since we clearly have $\langle u, u \rangle = \langle v, v \rangle$, we conclude that the above inequalities are all equalities. In particular, $\langle A_G u, u \rangle = \mu_1 \cdot \langle u, u \rangle$, hence u is an eigenvector corresponding to μ_1 by the exercise after Theorem 1.

The largest eigenvalue of A_G, cont'd

Since $u_i \geq 0$ for all i, it follows from the lemma that $u_i > 0$ for all i. We thus have an eigenvector corresponding to μ_1 with positive entries.
For the assertion in ii) we use a similar argument: suppose that $v' = (v'_1, \ldots, v'_n)$ is an eigenvector corresponding to μ_k and let $u' = (u'_1, \ldots, u'_n)$, where $u'_i = |v'_i|$. We thus have

$$|\mu_k| \cdot \langle v', v' \rangle = |\langle A_G v', v' \rangle| = \left| \sum_{i,j} a_{ij} v'_i v'_j \right|$$

$$\leq \sum_{i,j} a_{ij} u'_i u'_j = \langle A_G u', u' \rangle \leq \mu_1 \langle u', u' \rangle.$$

Since $\langle u', u' \rangle = \langle v', v' \rangle$, we conclude that $|\mu_k| \leq \mu_1$.

The largest eigenvalue of A_G, cont'd

Finally, in order to see that $\mu_1 > \mu_2$, we use the same trick one more time: if $\mu_1 = \mu_2$, then there is an eigenvector $\overline{v} = (\overline{v}_1, \ldots, \overline{v}_n) \in \mathbf{R}^n$ corresponding to μ_1, with $\langle u, \overline{v} \rangle = 0$, where u is a fixed eigenvector as in iii). If we define again $\overline{u} = (\overline{u}_1, \ldots, \overline{u}_n)$, with $\overline{u}_i = |\overline{v}_i|$, we see again that

$$\mu_1 \cdot \langle \overline{v}, \overline{v} \rangle = |\langle A_G \overline{v}, \overline{v} \rangle| = \left| \sum_{i,j} a_{i,j} \overline{v}_i \overline{v}_j \right|$$

$$\leq \sum_{i,j} a_{i,j} \overline{u}_i \overline{u}_j = \langle A_G \overline{u}, \overline{u} \rangle \leq \mu_1 \cdot \langle \overline{u}, \overline{u} \rangle.$$

Again, we see that these are all equalities. The second inequality becoming an equality implies that $\overline{u}$ is an eigenvector corresponding to μ_1. Since its entries are nonnegative, they are in fact positive by the lemma. In particular, we have $\overline{v}_i \neq 0$ for all i.

The largest eigenvalue of A_G, cont'd

The first inequality becoming an equality implies that all $\overline{v}_i\overline{v}_j$ with $a_{ij} > 0$ have the same sign. Since G is connected, it follows that all $\overline{v_j}$ have the same sign. This contradicts the fact that $\sum_i u_i\overline{v}_i = 0$.

Some references for what we are discussing about eigenvalues of graphs (and for a lot more):

Dan Spielman, Spectral Graph theory course, available at *http://cs.yale.edu/homes/spielman/561/2012/*

Lászlo Lovász, Eigenvalues of graphs, available at *https://web.cs.elte.hu/ lovasz/eigenvals-x.pdf*