

Lecture 12: Spectral graph theory

We introduce basic spectral graph theory today.

We will use it to analyze random walks, and also in graph partitioning and graph sparsification.

Eigenvalues and eigenvectors

Given an $n \times n$ matrix A , a nonzero vector v is an eigenvector of A if $Av = \lambda v$ for some scalar λ , which is called an eigenvalue associated with the eigenvector v .

The set of eigenvalues of A is given by the set of solutions to $\det(A - \lambda I) = 0$, the characteristic polynomial.

For an λ with $\det(A - \lambda I) = 0$, any vector $v \neq 0$ in the kernel/nullspace of $A - \lambda I$ is an associated eigenvector.

Real symmetric matrices

Our starting point of spectral graph theory is the following spectral theorem for real symmetric matrices.

Theorem. Let A be an $n \times n$ real symmetric matrix. Then there is an orthonormal basis of \mathbb{R}^n consisting of eigenvectors of A , and the corresponding eigenvalues are real numbers.

We will not prove this theorem; see e.g. the book "algebraic graph theory" by Godsil and Royle.

The above theorem applies to the adjacency matrices of undirected graphs, but not for directed graphs.

This is the main reason that spectral graph theory is much more developed for undirected graphs.

Let $v_1, v_2, \dots, v_n \in \mathbb{R}^n$ be the orthonormal basis of eigenvectors guaranteed by the above spectral theorem, with corresponding eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$.

Let V be the $n \times n$ matrix with the i -th column being v_i , i.e. $V = \begin{bmatrix} | & & | \\ v_1 & & v_n \\ | & & | \end{bmatrix}$.

Let D be the $n \times n$ diagonal matrix with the (i,i) -th entry being λ_i , i.e. $D = \begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \ddots \\ & & & \lambda_n \end{bmatrix}$.

Then the conditions $Av_i = \lambda_i v_i \quad \forall 1 \leq i \leq n$ can be compactly written as $AV = VD$.

Since the columns in V form an orthonormal basis, we have $V^T V = I$ and thus $V^{-1} = V^T$.

So, we can rewrite $AV = VD$ as $A = V D V^{-1} = V D V^T = \begin{bmatrix} | & & | \\ v_1 & & v_n \\ | & & | \end{bmatrix} \begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \ddots \\ & & & \lambda_n \end{bmatrix} \begin{bmatrix} -v_1- \\ \vdots \\ -v_n- \end{bmatrix}$.

This representation is very useful in computations.

Powers of matrices

To compute A^k , we observe that it is just $A^k = (V D V^T)^k = (V D V^T)(V D V^T) \dots (V D V^T) = V D^k V^T$ as $V^T V = I$.

Since D is a diagonal matrix, D^k is easy to compute, i.e. $D = \begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \ddots \\ & & & \lambda_n \end{bmatrix}$, $D^k = \begin{bmatrix} \lambda_1^k & & \\ & \lambda_2^k & \\ & & \ddots \\ & & & \lambda_n^k \end{bmatrix}$.

This is very useful, in analyzing random walks, as P^t is the transition matrix of the random walk after t steps where P is the transition matrix in one step.

We will use the eigenvalues of the transition matrix to bound the mixing time in a couple of lectures.

Eigen-decomposition

Since the eigenvectors form an orthonormal basis, any $x \in \mathbb{R}^n$ can be written uniquely as $c_1 v_1 + c_2 v_2 + \dots + c_n v_n$.

By orthonormality, $\langle x, v_i \rangle = \langle c_1 v_1 + \dots + c_n v_n, v_i \rangle = c_1 \langle v_1, v_i \rangle + \dots + c_i \langle v_i, v_i \rangle + \dots + c_n \langle v_n, v_i \rangle = c_i$.

Therefore, $x = \langle x, v_1 \rangle v_1 + \langle x, v_2 \rangle v_2 + \dots + \langle x, v_n \rangle v_n = v_1 v_1^T x + v_2 v_2^T x + \dots + v_n v_n^T x = (v_1 v_1^T + \dots + v_n v_n^T) x$.

This is true for all x , and hence $v_1 v_1^T + v_2 v_2^T + \dots + v_n v_n^T = I$, the identity matrix.

Multiplying both sides by A , we get $Ax = A(v_1 v_1^T + \dots + v_n v_n^T) x = (\lambda_1 v_1 v_1^T + \lambda_2 v_2 v_2^T + \dots + \lambda_n v_n v_n^T) x$.

This implies that $A = \lambda_1 v_1 v_1^T + \lambda_2 v_2 v_2^T + \dots + \lambda_n v_n v_n^T$, which can also be seen directly from $A = V D V^T$.

Finally, we claim that $A^{-1} = \frac{1}{\lambda_1} v_1 v_1^T + \frac{1}{\lambda_2} v_2 v_2^T + \dots + \frac{1}{\lambda_n} v_n v_n^T$ if $\lambda_i \neq 0$ for $1 \leq i \leq n$,

because $(\lambda_1 v_1 v_1^T + \dots + \lambda_n v_n v_n^T) \left(\frac{1}{\lambda_1} v_1 v_1^T + \dots + \frac{1}{\lambda_n} v_n v_n^T \right) = v_1 v_1^T + \dots + v_n v_n^T = I$.

Later on, we will use this idea to define the "pseudo-inverse" of A even when A is singular.

Positive semidefinite matrices

This is an important definition, an analog of a matrix being non-negative.

Fact Let A be a real symmetric matrix. The following statements are equivalent.

- ① A is positive semidefinite, i.e. all eigenvalues of A are non-negative.
- ② For any $x \in \mathbb{R}^n$, we have $x^T A x \geq 0$, i.e. all quadratic forms are non-negative.
- ③ $A = U^T U$ for some matrix $U \in \mathbb{R}^{n \times m}$.

proof Recall that a real symmetric matrix A can be written as $V D V^T$.

① \Rightarrow ③ Since all eigenvalues are non-negative, we can write $A = (V D^{\frac{1}{2}}) (D^{\frac{1}{2}} V^T)$ where $D^{\frac{1}{2}}$ is the $n \times n$ diagonal matrix with $D_{i,i} = \sqrt{\lambda_i}$.

Therefore, by letting $U = V D^{\frac{1}{2}}$, we see that A can be written as $U U^T$.

③ \Rightarrow ② $x^T A x = x^T U U^T x = \langle U^T x, U^T x \rangle = \|U^T x\|_2^2 \geq 0$ for any $x \in \mathbb{R}^n$.

② \Rightarrow ① We prove the contrapositive, \neg ① \Rightarrow \neg ②.

If v is an eigenvector with negative eigenvalue, then $v^T A v = \lambda v^T v = \lambda \|v\|_2^2 < 0$. \square

We will use the notation $A \succeq 0$ for A is a positive semidefinite matrix.

This is the basis of "semidefinite programming", a powerful generalization of linear programming.

Unfortunately, we will not be able to see it in this course.

Some identities

The following fact says that the sum of eigenvalues is equal to the trace of a matrix.

Fact Let $\lambda_1, \lambda_2, \dots, \lambda_n$ be the eigenvalues of $A \in \mathbb{R}^{n \times n}$. Then, $\sum_{i=1}^n \lambda_i = \text{trace}(A)$,

where $\text{trace}(A)$ is defined as the sum of diagonal entries of A , i.e. $\text{trace}(A) = \sum_{i=1}^n A_{ii}$.

Proof The proof is by considering the coefficients of $\det(\lambda I - A)$ as a polynomial in λ .

The roots of $\det(\lambda I - A)$ are the eigenvalues of A , and so $\det(\lambda I - A) = (\lambda - \lambda_1)(\lambda - \lambda_2) \dots (\lambda - \lambda_n)$.

Note that the coefficient of λ^{n-1} is $-\sum_{i=1}^n \lambda_i$.

On the other hand, $\det(\lambda I - A) = \det \begin{pmatrix} \lambda - a_{11} & -a_{12} & \dots & -a_{1n} \\ -a_{21} & \lambda - a_{22} & \dots & -a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ -a_{n1} & -a_{n2} & \dots & \lambda - a_{nn} \end{pmatrix}$.

By the Laplace expansion of the determinant, the coefficient of λ^{n-1} only appears in the term

$(\lambda - a_{11})(\lambda - a_{22}) \dots (\lambda - a_{nn})$, where the coefficient of λ^{n-1} in this term is $-\sum_{i=1}^n a_{ii}$.

Therefore, $\sum_{i=1}^n \lambda_i = \sum_{i=1}^n a_{ii} = \text{trace}(A)$. \square

We can use the same idea to derive other identities by writing other coefficients of $\det(\lambda I - A)$ in two ways. We won't need them and so leave as an exercise.

There is a nice identity for the product of the eigenvalues and the proof is left as an exercise

Fact $\det(A) = \prod_{i=1}^n \lambda_i$, where $\lambda_1, \dots, \lambda_n$ are the eigenvalues of A .

Graph spectrum

Spectral graph theory relates the combinatorial properties of a graph to the eigenvalues and eigenvectors of its associated matrix (e.g. adjacency matrix, Laplacian matrix).

Let's start with some examples and compute their spectrums.

Complete graph What is the spectrum of the complete graph on n vertices?

The adjacency matrix A is $J_n - I_n$, where J_n is the $n \times n$ all-one matrix.

Any vector is an eigenvector of I_n with eigenvalue 1.

Hence, the eigenvalues of A are just the eigenvalues of J_n minus one.

Since J_n is a rank one matrix, there are $n-1$ eigenvalues of 0, i.e. the eigenvalue 0 is of multiplicity $n-1$.

The all-one vector is an eigenvector of J_n with eigenvalue n , so the spectrum of J_n is $(n, 0, 0, \dots, 0)$.

So, A has one eigenvalue of $n-1$, and $n-1$ eigenvalues of -1 , so the spectrum of A is $(n-1, -1, -1, \dots, -1)$.

This is an example with the largest eigenvalue gap between the largest eigenvalue and the second largest.

Complete bipartite graph What is the spectrum of the complete bipartite graph $K_{m,n}$?

$m, n \in \mathbb{N}$

Complete bipartite graph What is the spectrum of the complete bipartite graph $K_{m,n}$?

The adjacency matrix A of $K_{m,n}$ looks like this:
$$\begin{matrix} m & \begin{matrix} \boxed{0} & \boxed{1} \\ \boxed{1} & \boxed{0} \end{matrix} \\ n & \end{matrix}$$

This matrix is of rank 2, so there are $n+m-2$ eigenvalues of 0, and two non-zero eigenvalues λ_1, λ_2 .

As $\sum_{i=1}^{n+m} \lambda_i = \text{trace}(A) = 0$, we have $\lambda_1 = -\lambda_2$. Let $\lambda_1 = k$ and we are to determine the value of k .

Then $\det(\lambda I - A) = (\lambda - \lambda_1)(\lambda - \lambda_2)\lambda^{n+m-2} = \lambda^{n+m} - k^2 \lambda^{n+m-2}$.

To determine k , we use the Laplace expansion of $\det \begin{pmatrix} \lambda & \lambda & \dots & -1 \\ \dots & \dots & \dots & \dots \\ -1 & \lambda & \dots & \lambda \end{pmatrix}$.

Any term that contributes to λ^{n+m-2} must have $n+m-2$ diagonal entries, and two off-diagonal entries $-a_{ij}, -a_{ji}$.

There are totally mn such terms, each contributing -1 to the coefficient of λ^{n+m-2} ,

as the sign of each term is -1 .

Therefore, $-k^2 = -mn$, and thus $k = \sqrt{mn}$.

To conclude, the spectrum of $K_{m,n}$ is $(\sqrt{mn}, 0, 0, \dots, 0, -\sqrt{mn})$.

Bipartite graphs Interestingly, we can characterize bipartite graphs by the spectrums.

The following lemma shows that the spectrum of a bipartite graph is symmetric around the origin.

Lemma If G is a bipartite graph and λ is an eigenvalue of $A(G)$ with multiplicity k , then $-\lambda$ is also an eigenvalue of $A(G)$ with multiplicity k .

Proof By permuting the rows and columns, we can write the adjacency of a bipartite graph as $A(G) = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}$.

Suppose $u = \begin{pmatrix} x \\ y \end{pmatrix}$ is an eigenvector of $A(G)$ with eigenvalue λ .

This implies that $\begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix}$, and hence $By = \lambda x$ and $B^T x = \lambda y$.

Consider the vector $\begin{pmatrix} x \\ -y \end{pmatrix}$.

Note that $\begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} x \\ -y \end{pmatrix} = \begin{pmatrix} -By \\ B^T x \end{pmatrix} = \begin{pmatrix} -\lambda x \\ \lambda y \end{pmatrix} = -\lambda \begin{pmatrix} x \\ -y \end{pmatrix}$, and so $\begin{pmatrix} x \\ -y \end{pmatrix}$ is an eigenvector of eigenvalue $-\lambda$.

Finally, k linearly independent eigenvectors of eigenvalue λ give k linearly independent eigenvectors of eigenvalue $-\lambda$ by the above construction, and so the multiplicity of λ and $-\lambda$ is the same. \square

We now prove that the converse is also true!

Lemma Let $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ be the eigenvalues of $A(G)$.

If $\lambda_i = -\lambda_{n-i+1}$ for $1 \leq i \leq n$, then G is a bipartite graph.

Proof Let $k \geq 1$ be an odd number.

Note that $\sum_{i=1}^n \lambda_i^k = 0$, by the symmetry of the spectrum.

Note also that $\lambda_1^k, \lambda_2^k, \dots, \lambda_n^k$ are the eigenvalues of A^k , because if $Au = \lambda u$ then $A^k u = \lambda^k u$.

By sum of eigenvalues equal trace, we have $\text{trace}(A^k) = \sum_{i=1}^n \lambda_i^k = 0$.

Observe that $A_{i,j}^k$ is equal to the number of length k walks from i to j in G (exercise by induction).

If G has an odd cycle of length k , then $A_{i,i}^k > 0$ for any vertex i in the cycle, hence $\text{trace}(A^k) > 0$.

Therefore, since $\text{trace}(A^k) = 0$, G must have no odd cycles and thus G is bipartite. \square

To conclude, we have a spectral characterization of a bipartite graph, that G is bipartite if and only if the spectrum of its adjacency matrix is symmetric around the origin.

Laplacian matrices

Given an undirected graph G , the Laplacian matrix $L(G)$ is defined as $D(G) - A(G)$, where

$D(G) = \begin{pmatrix} d_1 & & 0 \\ & d_2 & \\ 0 & & \ddots \\ & & & d_n \end{pmatrix}$ is the diagonal degree matrix with $D(G)_{ii} = \text{degree of vertex } i \text{ in } G$.

When G is a d -regular graph, then $D = dI$ and $L = dI - A$. Thus any eigenvector of A with eigenvalue λ is an eigenvector of L with eigenvalue $d - \lambda$, and vice versa.

So, in this case the spectrums of the adjacency matrix and the Laplacian matrix are basically equivalent, but when G is non-regular it may not be so easy to relate their eigenvalues.

Let's try to understand more about the spectrum of the Laplacian matrices.

Let $\vec{1}$ be the all-one vector. Then it is easy to check that $L\vec{1} = \vec{0}$.

So, $L(G)$ has 0 as an eigenvalue for any graph G .

Can $L(G)$ have a smaller eigenvalue (i.e. a negative eigenvalue)?

Let $e = ij$ be an edge in G . Let the Laplacian of edge be $L_e = \begin{matrix} & i & j \\ \begin{matrix} + & - \\ - & + \end{matrix} & & \end{matrix}$ (with only 4 nonzero entries).

Then, it can be checked that $L(G) = L(G - e) + L_e$, and it follows by induction that $L(G) = \sum_{e \in E} L_e$.

For $e = ij$, let $b_e \in \mathbb{R}^n$ be the column vector with the i -th entry equal +1 and the j -th entry equal -1 and zero o.w.

Then, it is easy to see that $L_e = \begin{bmatrix} +1 & -1 \\ -1 & +1 \end{bmatrix} = \begin{bmatrix} +1 \\ -1 \end{bmatrix} \begin{bmatrix} +1 & -1 \end{bmatrix} = b_e b_e^T$, and thus L_e is a positive semidefinite matrix.

This implies that L is also a positive semidefinite matrix, as a sum of PSD matrices is also a PSD matrix.

Therefore, 0 is the smallest eigenvalue of $L(G)$ for any G .

One advantage of the Laplacian matrix is that we know its smallest eigenvalue and its corresponding eigenvector $\vec{1}$.

Connectedness

It turns out that the smallest eigenvalue of $L(G)$ gives a spectral characterization of whether G is connected.

Proposition A graph G is connected if and only if 0 is an eigenvalue of $L(G)$ with multiplicity one.

Proof If G is disconnected, then the vertex set can be partitioned into two sets S_1 and S_2

such that there are no edges between them. Then, $L(G) = \begin{pmatrix} L(G_1) & 0 \\ 0 & L(G_2) \end{pmatrix}$, and so

$\begin{pmatrix} 1 \\ \vdots \\ 0 \\ \vdots \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}$ are both eigenvectors of $L(G)$ with eigenvalue 0, hence of multiplicity ≥ 2 .

If G is connected, consider $x^T L x = x^T \left(\sum_{e \in E} L_e \right) x = \sum_{e \in E} x^T L_e x = \sum_{e \in E} x^T b_e b_e^T x = \sum_{e \in E} (x_i - x_j)^2 \geq 0$

If x is an eigenvector of eigenvalue 0, then $x^T L x = 0$.

For $x^T L x = \sum_{e \in E} (x_i - x_j)^2 = 0$, it must hold that $x_i = x_j$ for all $ij \in E$.

Since G is connected, it follows that $x_i = x_j$ for all $i, j \in V$, and thus $x = c \vec{1}$ for some value $c \in \mathbb{R}$.

Therefore, all eigenvectors of eigenvalue 0 live in a one-dimensional subspace (spanned by the vector $\vec{1}$),

and thus 0 is an eigenvalue of multiplicity 1. \square

We usually order the eigenvalues of a Laplacian matrix as $0 = \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$.

Then the above result says that G is connected if and only if $\lambda_2 > 0$ (or G disconnected iff $\lambda_2 = 0$).

The statement can be generalized as follows. The proof is left as an exercise.

Proposition A graph G has k connected components if and only if the k -th smallest eigenvalue of its Laplacian matrix is equal to zero.

Generalizations

So far we have seen some spectral characterizations of combinatorial properties of a graph, such as bipartiteness and connectedness, but these are simple properties that are easy to deduce by other methods.

The key feature of these spectral characterizations is that they can be generalized nontrivially and quantitatively:

- λ_2 is "small" iff the graph is "close" to be disconnected (i.e. the existence of a "sparse" cut).
- λ_k is "small" iff the graph is "close" to having k components (i.e. k disjoint "sparse" cuts).
- α_n is "close" to $-\alpha_1$ (adjacency matrix) iff the graph has a "close-to-bipartite-component".

We will prove the first item and mention the next two items in the next lecture.

Rayleigh Quotient

The main concept in relating eigenvalues and eigenvectors to optimization problems is the Rayleigh quotient,

which is defined as $\frac{x^T A x}{x^T x} = \frac{\sum_{i,j} a_{ij} x_i x_j}{\sum_i x_i^2}$, i.e. the quadratic form normalized by the squared length.

Let A be a real symmetric matrix with eigenvalues $\alpha_1 \geq \alpha_2 \geq \dots \geq \alpha_n$, and orthonormal eigenvectors v_1, v_2, \dots, v_n .

Lemma $\alpha_1 = \max_x \frac{x^T A x}{x^T x}$

Proof Let $x = c_1 v_1 + c_2 v_2 + \dots + c_n v_n$, as v_1, \dots, v_n form a basis.

$$\begin{aligned} \text{Then } x^T A x &= (c_1 v_1 + \dots + c_n v_n)^T A (c_1 v_1 + \dots + c_n v_n) \\ &= (c_1 v_1 + \dots + c_n v_n)^T (c_1 \alpha_1 v_1 + c_2 \alpha_2 v_2 + \dots + c_n \alpha_n v_n) \\ &= \sum_{i=1}^n c_i^2 \alpha_i \quad (\text{as } v_1, \dots, v_n \text{ are orthonormal}) \end{aligned}$$

Similarly, $x^T x = (c_1 v_1 + \dots + c_n v_n)^T (c_1 v_1 + \dots + c_n v_n) = \sum_{i=1}^n c_i^2$.

$$\text{So, } \frac{x^T A x}{x^T x} = \frac{\sum_{i=1}^n c_i^2 \alpha_i}{\sum_{i=1}^n c_i^2} \leq \frac{\alpha_1 \sum_{i=1}^n c_i^2}{\sum_{i=1}^n c_i^2} = \alpha_1.$$

Since v_1 attains the maximum, the lemma follows. \square

This can be used to characterize other eigenvalues.

Let T_k be the set of vectors that are orthogonal to v_1, \dots, v_{k-1} .

Lemma $\alpha_k = \max_{x \in T_k} \frac{x^T A x}{x^T x}$

Proof Let $x \in T_k$. Write $x = c_1 v_1 + \dots + c_n v_n$.

Recall that $c_i = \langle x, v_i \rangle$. Since $x \in T_k$, it follows that $c_1 = c_2 = \dots = c_{k-1} = 0$.

$$\text{Then, } \frac{x^T A x}{x^T x} = \frac{\sum_{i=k}^n c_i^2 \alpha_i}{\sum_{i=k}^n c_i^2} \leq \frac{\alpha_k \sum_{i=k}^n c_i^2}{\sum_{i=k}^n c_i^2} = \alpha_k.$$

Since $v_k \in T_k$ and $\frac{v_k^T A v_k}{v_k^T v_k} = \alpha_k$, the lemma follows. \square

The above result gives a characterization of α_k , but it requires the knowledge of the previous eigenvectors.

The following result gives a characterization without using T_k , and this is useful in providing bounds on eigenvalues.

Courant-Fischer Theorem $\alpha_k = \max_{\substack{S \subseteq \mathbb{R}^n \\ \dim(S)=k}} \min_{x \in S} \frac{x^T A x}{x^T x} = \min_{\substack{S \subseteq \mathbb{R}^n \\ \dim(S)=n-k+1}} \max_{x \in S} \frac{x^T A x}{x^T x}$

Proof (Optional) We first consider the max-min term.

Let S_k be the k -dimensional subspace spanned by v_1, \dots, v_k , i.e. $\{x \mid x = c_1 v_1 + \dots + c_k v_k \text{ for some } c_1, \dots, c_k\}$.

$$\text{For any } x \in S_k, \frac{x^T A x}{x^T x} = \frac{(c_1 v_1 + \dots + c_k v_k)^T A (c_1 v_1 + \dots + c_k v_k)}{(c_1 v_1 + \dots + c_k v_k)^T (c_1 v_1 + \dots + c_k v_k)} = \frac{\sum_{i=1}^k c_i^2 \alpha_i}{\sum_{i=1}^k c_i^2} \geq \frac{\alpha_k \sum_{i=1}^k c_i^2}{\sum_{i=1}^k c_i^2} = \alpha_k.$$

$$\text{So, } \max_{\substack{S \subseteq \mathbb{R}^n \\ \dim(S)=k}} \min_{x \in S} \frac{x^T A x}{x^T x} \geq \min_{x \in S_k} \frac{x^T A x}{x^T x} \geq \alpha_k.$$

To prove that the maximum cannot be greater than α_k , observe that any k -dimensional subspace must intersect the $n-k+1$ dimensional subspace T_k spanned by $\{v_k, v_{k+1}, \dots, v_n\}$.

$$\text{For any } x \in T_k, \frac{x^T A x}{x^T x} = \frac{\sum_{i=k}^n c_i^2 \alpha_i}{\sum_{i=k}^n c_i^2} \leq \alpha_k.$$

$$x^T x = \sum_{i=1}^n c_i^2 = \dots$$

$$So, \max_{S \subseteq R, \dim(S)=k} \min_{x \in S} \frac{x^T A x}{x^T x} \leq \max_{S \subseteq R, \dim(S)=k} \min_{x \in S \cap T_k} \frac{x^T A x}{x^T x} \leq \alpha_k. \quad \square$$

Largest eigenvalue of adjacency matrix

Let A be the adjacency matrix of an undirected graph. Let α_1 be its largest eigenvalue.

Claim $\alpha_1 \leq d_{\max}$, where d_{\max} denotes the maximum degree in G .

Proof Let v_1 be an eigenvector with eigenvalue α_1 .

Let j be the vertex with $v_1(j) \geq v_1(i)$ for all i .

$$\text{Then, } \alpha_1 v_1(j) = (A v_1)(j) = \sum_{i: ij \in E(G)} v_1(i) \leq \sum_{i: ij \in E(G)} v_1(j) = \deg(j) \cdot v_1(j) \leq d_{\max} \cdot v_1(j).$$

Therefore, $\alpha_1 \leq d_{\max}$. \square

When $\lambda_1 = d_{\max}$, then the above inequalities must hold as equalities, i.e. $v_1(i) = v_1(j)$ for every neighbor i of j and also $\deg(j) = d_{\max}$. So, when G is connected and $\lambda_1 = d_{\max}$, then G must be d_{\max} -regular and the eigenvalue λ_1 is of multiplicity one.

The Perron-Frobenius theorem for non-negative matrices tell us more about the first eigenvalue and eigenvector.

Theorem Let G be a connected undirected graph. Then,

- ① the first eigenvalue is of multiplicity one.
- ② $|\alpha_i| \leq \alpha_1$ for all i .
- ③ all entries of the first eigenvector are nonzero and have the same sign.

We will not prove it. See chapter 8 of "Algebraic graph theory" by Godsil and Royle for proofs.

References

- Lecture notes of "spectral graph theory" by Dan Spielman (and an upcoming book).
- "Algebraic graph theory" by Godsil and Royle.