4.1 Eigenvalues and Optimization

I cannot believe that I have managed to teach three lectures on spectral graph theory without giving the characterization of eigenvalues as solutions to optimization problems. It is one of the most useful ways of understanding eigenvalues of symmetric matrices.

To begin, let $A$ be a symmetric matrix with eigenvalues

$$\alpha_1 \geq \alpha_2 \geq \cdots \geq \alpha_n,$$

and corresponding orthonormal eigenvectors $v_1, \ldots, v_n$.

**Lemma 4.1.1.**

$$\alpha_1 = \max_x \frac{x^T Ax}{x^T x}.$$

The ratio on the right-hand side of this expression is called the *Rayleigh quotient* of $x$ with respect to $A$.

**Proof.** As the eigenvectors provide an orthonormal basis, we may expand $x$ in this basis to obtain

$$x = \sum_i c_i v_i, \quad \text{where} \quad c_i = v_i^T x.$$

We then have

$$x^T A x = \left( \sum_i c_i v_i \right)^T A \left( \sum_i c_i v_i \right)$$

$$= \left( \sum_i c_i v_i \right)^T \left( \sum_i \alpha_i c_i v_i \right)$$

$$= \sum_i c_i^2 \alpha_i,$$

where in the last equality we have exploited the orthonormality of the vectors $v_1, \ldots, v_n$. Similarly, we have

$$x^T x = \left( \sum_i c_i v_i \right)^T \left( \sum_i c_i v_i \right) = \sum_i c_i^2.$$
So, for every \( x \)

\[
\frac{x^T A x}{x^T x} = \frac{\sum_i c_i^2 \alpha_i}{\sum_i c_i^2} \leq \frac{\sum_{i=k}^n c_i^2 \alpha_i}{\sum_{i=k}^n c_i^2} = \alpha_k \frac{\sum_{i=k}^n c_i^2}{\sum_{i=k}^n c_i^2} = \alpha_1.
\]

Observe that the maximum of \( \alpha_1 \) is actually achieved by \( x = v_1 \). \( \square \)

We may similarly characterize the other eigenvalues. The \( k \)th eigenvalue is obtained by taking the maximum over vectors orthogonal to \( v_1, \ldots, v_{k-1} \):

**Lemma 4.1.2.** Let \( T_k \) be the space of vectors orthogonal to \( v_1, \ldots, v_{k-1} \). Then,

\[
\alpha_k = \max_{x \in T_k} \frac{x^T A x}{x^T x}.
\]

**Proof.** First observe that the value of \( \alpha_k \) is achieved by setting \( x = v_k \). Next, expand \( x \) in the basis of eigenvectors as before, but exploit the fact that \( x^T v_i = c_i = 0 \), for \( i \leq k \). So, for every \( x \) orthogonal to \( v_1, \ldots, v_{k-1} \),

\[
\frac{x^T A x}{x^T x} = \frac{\sum_{i=k}^n c_i^2 \alpha_i}{\sum_{i=1}^n c_i^2} = \frac{\sum_{i=k}^n c_i^2 \alpha_i}{\sum_{i=k}^n c_i^2} \leq \alpha_k \frac{\sum_{i=k}^n c_i^2}{\sum_{i=k}^n c_i^2} = \alpha_1.
\]

\( \square \)

### 4.2 Graph Coloring and \( \alpha_1 \)

Last class, we proved that for the adjacency matrix \( A_G \) of a graph \( G \), \( \alpha_1 \) is at most the maximum degree of a vertex in \( G \). Lemma 4.1.1 provides an easy way of proving a lower bound on \( \alpha_1 \): just compute the Rayleigh quotient for some vector \( x \).

**Lemma 4.2.1.** Let \( A_G \) be the adjacency matrix of an unweighted graph \( G \). Then \( \alpha_1 \) is at least the average degree of the vertices in \( G \).

**Proof.** Let \( d \) denote the vector of degrees of vertices in \( G \), so \( d(i) \) is the degree of vertex \( i \). Now, take the Rayleigh quotient of the all-1s vector. We find

\[
\alpha_1 = \max_x \frac{x^T A x}{x^T x} \geq \frac{1^T A 1}{1^T 1} = \frac{1^T d}{n} = \frac{1}{n} \sum_i d(i).
\]

\( \square \)

While we may think of \( \alpha_1 \) as being related to the average degree, it does behave differently. In particular, if we remove the vertex of smallest degree from a graph, the average degree can increase. On the other hand, \( \alpha_1 \) can only decrease when we remove a vertex. Let’s prove that now.

**Lemma 4.2.2.** Let \( A \) be a symmetric matrix, let \( B \) be the matrix obtained by removing the last row and column from \( A \), and let \( \beta_1 \) be the largest eigenvalue of \( B \). Then,

\[
\alpha_1 \geq \beta_1.
\]
Proof. For any vector \( y \in \mathbb{R}^{n-1} \), we have

\[
y^T B y = \begin{pmatrix} y \\ 0 \end{pmatrix}^T A \begin{pmatrix} y \\ 0 \end{pmatrix}.
\]

So, for \( y \) an eigenvector of \( B \) of eigenvalue \( \beta_1 \),

\[
\beta_1 = \frac{y^T B y}{y^T y} = \frac{\begin{pmatrix} y \\ 0 \end{pmatrix}^T A \begin{pmatrix} y \\ 0 \end{pmatrix}}{\begin{pmatrix} y \\ 0 \end{pmatrix}^T \begin{pmatrix} y \\ 0 \end{pmatrix}} \leq \max_{x \in \mathbb{R}^n} \frac{x^T A x}{x^T x}.
\]

Of course, this holds regardless of which row and column we remove, as long as they are the same row and column.

Recall that a \( k \)-coloring of a graph \( G = (V, E) \) is a function \( c : V \to \{1, \ldots, k\} \) such that

\[
c(i) \neq c(j), \text{ for all } (i, j) \in E.
\]

The **chromatic number** of a graph \( G \), written \( \chi(G) \), is the least \( k \) for which \( G \) has a \( k \)-coloring. We will now prove a theorem of Wilf.

**Theorem 4.2.3.**

\[
\chi(G) \leq \lceil \alpha_1 \rceil + 1.
\]

**Proof.** We prove this by induction on the number of vertices in the graph. To ground the induction, consider the graph with one vertex and no edges. It has chromatic number 1 and largest eigenvalue zero\(^1\). Now, assume the theorem is true for all graphs on \( n - 1 \) vertices, and let \( G \) be a graph on \( n \) vertices. By Lemma 4.2.1, \( G \) has a vertex of degree at most \( \lceil \alpha_1 \rceil \). Let \( v \) be such a vertex and let \( G - \{v\} \) be the graph obtained by removing this vertex. By Lemma 4.2.2 and our induction hypothesis, \( G - \{v\} \) has a coloring with at most \( \lceil \alpha_1 \rceil + 1 \) colors. Let \( c \) be any such coloring. We just need to show that we can extend \( c \) to \( v \). As \( v \) has at most \( \lceil \alpha_1 \rceil \) neighbors, there is some color in \( \{1, \ldots, \lceil \alpha_1 \rceil + 1\} \) that does not appear among its neighbors, and which it may be assigned. Thus, \( G \) has a coloring with \( \lceil \alpha_1 \rceil + 1 \) colors. \( \square \)

This is an improvement over the classical result \( \chi \leq d_{\text{max}} + 1 \), as there are graphs for which \( \alpha_1 \) is much less than \( d_{\text{max}} \). For example, for a path graph with at least 3 vertices, we have \( d_{\text{max}} = 2 \), but \( \alpha_1 < 2 \).

\(^1\)If this makes you uncomfortable, you could use both graphs on two vertices
4.3 The Courant-Fischer Theorem

I gave a hint of the Courant-Fischer Theorem earlier in the lecture. I’ll do the rest of it now.

**Theorem 4.3.1** (Courant-Fischer Theorem). Let $A$ be a symmetric matrix with eigenvalues $\alpha_1 \geq \alpha_2 \geq \cdots \geq \alpha_n$. Then,

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

For example, consider the case $k = 1$. In this case, $S$ is just the span of $v_1$ and $T$ is all of $\mathbb{R}^n$. For general $k$, the optima will be achieved when $S$ is the span of $v_1, \ldots, v_k$ and when $T$ is the span of $v_k, \ldots, v_n$.

**Proof.** We will just verify the first characterization of $\alpha_k$. The other is similar.

First, let’s verify that $\alpha_k$ is achievable. Let $S_k$ be the span of $v_1, \ldots, v_k$. For every $x \in S_k$, we can write

$$x = \sum_{i=1}^k c_i v_i,$$

so, as before,

$$\frac{x^T A x}{x^T x} = \sum_{i=1}^k \frac{\alpha_i c_i^2}{c_i^2} \geq \sum_{i=1}^k \frac{\alpha_k c_i^2}{c_i^2} = \alpha_k.$$

To verify that this is in fact the maximum, let $T_k$ be the span of $v_k, \ldots, v_n$. As $T_k$ has dimension $n-k+1$, for any $S$ of dimension $k$ the intersection of $S$ with $T_k$ is non-empty. So,

$$\min_{x \in S \cap T_k} \frac{x^T A x}{x^T x} \leq \min_{x \in S} \frac{x^T A x}{x^T x}.$$

Any such $x$ may be expressed as

$$x = \sum_{i=k}^n c_i v_i,$$

and so

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

We conclude that for all subspaces $S$ of dimension $k$,

$$\min_{x \in S} \frac{x^T A x}{x^T x} \leq \alpha_k.$$

We can finally derive Sylvester’s Law of Interia.
**Theorem 4.3.2** (Sylvester’s Law of Intertia). Let $A$ be any symmetric matrix and let $B$ be any non-singular matrix. Then, the matrix $BAB^T$ has the same number of positive, negative and zero eigenvalues as $A$.

**Proof.** It is clear that $A$ and $BAB^T$ have the same rank, and thus the same number of zero eigenvalues.

We will prove that $A$ has at least as many positive eigenvalues as $BAB^T$. As $B$ is invertible, we may switch the roles of $A$ and $BAB^T$ in the proof, and prove that $BAB^T$ has at least as many positive eigenvalues as does $A$. Thus, they have the same number of positive eigenvalues. The negative eigenvalues may be handled similarly.

Let $\gamma_1, \ldots, \gamma_k$ be the positive eigenvalues of $BAB^T$ and let $Y_k$ be the span of the corresponding eigenvectors. Now, let $S_k$ be the span of the vectors $B^Ty$, for $y \in Y_k$. As $B$ is non-singular, $S_k$ has dimension $k$. By Theorem 4.3.1, we have

$$\alpha_k = \max_{S \subseteq \mathbb{R}^n \text{ dim}(S) = k} \min_{x \in S} \frac{x^T A x}{x^T x} \geq \min_{x \in S_k} \frac{x^T A x}{x^T x} = \min_{y \in Y_k} \frac{y^T BAB^T y}{y^T y} > 0.$$ 

So, $A$ has at least $k$ positive eigenvalues.

**4.4 Independent Sets**

Hoffman was the first to observe a connection between the chromatic number and the smallest eigenvalue of the adjacency matrix. His proof goes through the independence number of a graph. Recall that $W \subseteq V$ is an independent set of vertices if there are no edges between vertices in $W$. We denote the size of the largest independent set by $\alpha(G)$. In a coloring of a graph, each color class must be an independent set. So,

$$\chi(G) \geq \frac{n}{\alpha(G)}.$$ 

The key fact about independent sets that we will exploit in our proof is that if $S$ is an independent set and $\chi_S$ is its characteristic vector\(^2\), then

$$\chi_S^T A \chi_S = 0.$$ 

**Theorem 4.4.1.** Let $G = (V, E)$ be a $d$-regular graph. Then

$$\alpha(G) \leq n \frac{-\alpha_n}{d - \alpha_n}.$$ 

As the trace of the adjacency matrix is 0, $\alpha_n$ is negative. So, this has the right sign.

\(^2\)That is, $\chi_S(i)$ is 1 if $i \in S$ and 0 otherwise.
Proof. As usual $\alpha_1 \geq \alpha_2 \geq \cdots \geq \alpha_n$ be the eigenvalues of $A_G$ and let $v_1, \ldots, v_n$ be the corresponding eigenvectors. Recall that $\alpha_1 = d$, $v_1 = 1/\sqrt{n}$, and that all other eigenvectors are orthogonal to $v_1$. Let $J$ be the matrix all of whose entries are 1. We have

$$Jv_i = \begin{cases} \ n v_1 & \text{for } i = 1 \\ 0 & \text{for } i \geq 2. \end{cases}$$

Now, consider the matrix

$$B = A - cJ,$$

where we will set $c = \frac{d - \alpha_n}{n}$.

We can compute the eigenvalues of $B$ from

$$Bv_i = \begin{cases} \ (d - cn)v_1 & \text{for } i = 1 \\ \alpha_i v_i & \text{for } i \geq 2. \end{cases}$$

We have chosen $c$ so that the smallest eigenvalue of $B$ is $d - cn = \alpha_n$.

On the other hand, let $S$ be an independent set of vertices in $G$, and let $\chi_S$ be the characteristic vector of this set. As $S$ is independent in $G$,

$$\chi^T_S A \chi_S = 0.$$

So,

$$\chi^T_S B \chi_S = \chi^T_S A \chi_S - c \chi^T_S J \chi_S = -c |S|^2,$$

and

$$\frac{\chi^T_S B \chi_S}{\chi^T_S \chi_S} = \frac{-c |S|^2}{|S|} = -c |S|.$$

The Courant-Fischer theorem tells us that this is larger than the smallest eigenvalue of $B$, so

$$\alpha_n \leq -c |S| = \frac{\alpha_n - d}{n} |S|,$$

which implies

$$n \frac{-\alpha_n}{d - \alpha_n} \geq |S|.$$

For example, consider a ring graph on $n$ vertices. For $n$ even, we have $d = 2$ and $\alpha_n = -2$, which provides the upper bound $\alpha(G) \leq n/2$. For $n$ odd, we have $\alpha_n > -2$, so we find $\alpha(G) < n/2$.

We obtain the following bound on the chromatic number of a $d$-regular graph:

$$\chi(G) \geq \frac{n}{\alpha(G)} \geq \frac{d - \alpha_n}{-\alpha_n} = 1 + \frac{d}{-\alpha_n}.$$
For the ring graph on an odd number of vertices, we have $\alpha_n > -2$ and so we can show $\chi(G) > 2$.

Note that the proof of Theorem 4.4.1 breaks down for irregular graphs. The problem is that $J$ is no longer proportional to $v_1v_1^T$. In many proofs in spectral graph theory, one fixes this by replacing $J$ with $v_1v_1^T$. However, we would then no longer know the value of $\chi^T_S(v_1v_1^T)\chi_S$.

4.5 Hoffman’s Bound

The last bound on the chromatic number holds even for irregular graphs.

**Theorem 4.5.1.**

$$\chi(G) \geq \frac{\alpha_1 - \alpha_n}{-\alpha_n} = 1 + \frac{\alpha_1}{-\alpha_n}.$$  

In fact, this theorem holds for arbitrary weighted graphs, if we substitute $\alpha$ for $d$. Thus, one may prove lower bounds on the chromatic number of a graph by assigning a weight to every edge, and computing the resulting ratio. However, we will not have time to prove this in class. I may add a proof to these notes for your reference.

We begin with a useful fact about the eigenvalues of block-partitioned matrices. Please let me know if you can find a better proof of this.

In this section, I will let $\lambda_{\text{max}}(A)$ and $\lambda_{\text{min}}(A)$ denote the largest and smallest eigenvalues of the matrix $A$.

**Lemma 4.5.2.** Let 

$$A = \begin{bmatrix} B & C \\ C^T & D \end{bmatrix}$$

be a symmetric matrix. Then 

$$\lambda_{\text{min}}(A) + \lambda_{\text{max}}(A) \leq \lambda_{\text{max}}(B) + \lambda_{\text{max}}(D).$$

**Proof.** Let $x$ be an eigenvector of $A$ of eigenvalue $\lambda_{\text{max}}(A)$. To simplify formulae, let’s also assume that $x$ is a unit vector. Write $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$, using the same partition as we did for $A$. Set 

$$y = \begin{pmatrix} \|x_2\| \frac{x_1}{\|x_1\|} \\ -\|x_1\| \frac{x_2}{\|x_2\|} \end{pmatrix}.$$ 

The reader may verify that $y$ is also a unit vector. By the Courant-Fischer Theorem, 

$$y^T A y \geq \lambda_{\text{min}}(A).$$
We have
\[ \lambda_{\text{max}}(A) + \lambda_{\text{min}}(A) \leq x^T A x + y^T A y \]
\[ = x_1^T B x_1 + x_1^T C x_2 + x_2^T C^T x_1 + x_2^T D x_2 + \]
\[ + \frac{\|x_2\|^2}{\|x_1\|^2} x_1^T B x_1 - x_1^T C x_2 - x_2^T C^T x_1 + \frac{\|x_1\|^2}{\|x_2\|^2} x_2^T D x_2 \]
\[ = x_1^T B x_1 + x_2^T D x_2 + \frac{\|x_2\|^2}{\|x_1\|^2} x_1^T B x_1 + \frac{\|x_1\|^2}{\|x_2\|^2} x_2^T D x_2 \]
\[ \leq \left( 1 + \frac{\|x_2\|^2}{\|x_1\|^2} \right) x_1^T B x_1 + \left( 1 + \frac{\|x_1\|^2}{\|x_2\|^2} \right) x_2^T D x_2 \]
\[ = \lambda_{\text{max}}(B) \left( \|x_1\|^2 + \|x_2\|^2 \right) + \lambda_{\text{max}}(D) \left( \|x_1\|^2 + \|x_2\|^2 \right) \]
\[ = \lambda_{\text{max}}(B) + \lambda_{\text{max}}(D), \]
as \( x \) is a unit vector.

**Lemma 4.5.3.** Let

\[
A = \begin{bmatrix}
    A_{1,1} & A_{1,2} & \cdots & A_{1,k} \\
    A_{1,2}^T & A_{2,2} & \cdots & A_{2,k} \\
    \vdots & \vdots & \ddots & \vdots \\
    A_{1,k}^T & A_{2,k}^T & \cdots & A_{k,k}
\end{bmatrix}
\]

be a block-partitioned symmetric matrix with \( k \geq 2 \). Then

\[ (k - 1) \lambda_{\text{min}}(A) + \lambda_{\text{max}}(A) \leq \sum_i \lambda_{\text{max}}(A_{i,i}). \]

**Proof.** For \( k = 2 \), this is exactly Lemma 4.5.2. For \( k > 2 \), we apply induction. Let

\[
B = \begin{bmatrix}
    A_{1,1} & A_{1,2} & \cdots & A_{1,k-1} \\
    A_{1,2}^T & A_{2,2} & \cdots & A_{2,k-1} \\
    \vdots & \vdots & \ddots & \vdots \\
    A_{1,k-1}^T & A_{2,k-1}^T & \cdots & A_{k-1,k-1}
\end{bmatrix}
\]

As we did in the proof of Lemma 4.2.2, we can use the Courant-Fischer Theorem to prove that

\[ \lambda_{\text{min}}(B) \geq \lambda_{\text{min}}(A). \]

Applying Lemma 4.5.2 to \( B \) and the \( k \)th row and column of \( A \), we find

\[ \lambda_{\text{min}}(A) + \lambda_{\text{max}}(A) \leq \lambda_{\text{max}}(B) + \lambda_{\text{max}}(A_{k,k}) \]
\[ \leq -(k - 2) \lambda_{\text{min}}(B) + \sum_{i=1}^{k-1} \lambda_{\text{max}}(A_{i,i}) + \lambda_{\text{max}}(A_{k,k}) \quad \text{(by induction)} \]
\[ \leq -(k - 1) \lambda_{\text{min}}(A) + \sum_{i=1}^{k} \lambda_{\text{max}}(A_{i,i}), \]
which proves the lemma.
Proof of Theorem 4.5.1. Let $G$ be a $k$-colorable graph. After possibly re-ordering the vertices, the adjacency matrix of $G$ can be written

$$
\begin{bmatrix}
0 & A_{1,2} & \cdots & A_{1,k} \\
A_{1,2}^T & 0 & \cdots & A_{2,k} \\
\vdots & \vdots & \ddots & \vdots \\
A_{i,k}^T & A_{2,k}^T & \cdots & 0 \\
\end{bmatrix}
$$

As each diagonal block is all-zero, Lemma 4.5.3 implies

$$(k-1)\lambda_{\min}(A) + \lambda_{\max}(A) \leq 0.$$  

Recalling that $\lambda_{\min}(A) = \alpha_n < 0$, and $\lambda_{\max}(A) = \alpha_1$, a little algebra yields

$$1 + \frac{\alpha_1}{-\alpha_n} \leq k.$$  

$\square$