SUM OF THE LARGEST EIGENVALUES OF SYMMETRIC MATRICES AND GRAPHS

by

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Abstract

D. Gernert conjectured that the sum of two largest eigenvalues of the adjacency matrix of a simple graph is at most the number of vertices of the graph. This can be proved, in particular, for all regular graphs. Gernert's conjecture was recently disproved by Nikiforov, who also provided a nontrivial upper bound for the sum of two largest eigenvalues. We will study extensions of these results to general $n \times n$ symmetric matrices with entries from $[0, 1]$ and try to improve Nikiforov's theorem. We will also study other recent results on the extreme behavior of the sum the k largest eigenvalues of symmetric matrices and particularly, adjacency matrices of graphs.

Keywords:
eigenvalue, eigenvector, spectrum of graphs.

To my dearest parents,
and my beloved wife, Narges

"What we know is a drop, what we don't know, an ocean."

— *Isaac Newton*

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Introduction and background

1.1 Introduction

Mathematical chemistry is a novel area of research which deals with applications of mathematics to chemistry. It mainly concerns with modeling of the chemical objects and phenomena. This area is involved with different and wide areas of mathematics. Group theory, Graph theory and in particular spectral graph theory and topology are just examples of these areas. There is more information about this subject in [13].

An example of such modeling is the modeling of molecules with graphs. In fact, for any atom in a molecule, we can assign a vertex and join two vertices by an edge if there is a chemical bond between the corresponding atoms. It turns out that some of the chemical parameters of this atom can be estimated by some of the parameters of its graph such as the spectrum of the graph.

There is a variety of mathematical questions which arise from these kind of modeling. In some cases, the questions are already answered and in some other cases they become research problem for mathematicians. In this thesis we will consider a problem of the second kind.

Let G be a graph of order n with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Define $L_k(G) = \lambda_1 + \lambda_2 + \cdots + \lambda_k$ where $1 \leq k \leq n$. Gernert [7] posed the following question: Is $L_2(G) \leq n$ for any graph G of order n? He showed that the answer is positive for the following types of graphs: regular graphs, triangle free graphs, toroidal graphs and planar graphs and also all the graphs on at most 10 vertices. Then he conjectured that the same result is valid for any simple graph. In Chapter 3 we will show that Gernert's result about regular graphs holds in a more general setting.

In 2006, Nikiforov [17] disproved Gernert's conjecture by exhibiting a graph G of order n with $L_2(G) \geq \frac{29+\sqrt{329}}{42}n - 25 \approx 1.122n - 25$ for any $n \geq 21$. Furthermore, he proved that $L_2(G) \leq \frac{2}{\sqrt{3}}n$ for any graph G of order n. A year after, Ebrahimi, Mohar, and Sheikh Ahmady [5], independently, constructed simpler counterexamples to Gernert's conjecture with $L_2(G) \geq \frac{8}{7}n \approx 1.14n$ for any $n \equiv 0 \pmod 7$. They also generalized Nikiforov's result on the upper bound on $L_2(G)$ for a more general class of matrices. We will discuss these results in Chapter 3 in detail.

In 2007, Mohar [16] posed the following generalization of Gernert's problem. Let $\mathcal{M}_n$ be the set of all symmetric matrices of size n with entries from the interval [0,1]. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of $A \in \mathcal{M}_n$. Let $L_k(A) = \lambda_1 + \lambda_2 + \cdots + \lambda_k$. For $1 \leq k \leq n$ define

$$\tau_k(n) = \frac{1}{n}\sup\{L_k(A) \mid A \in \mathcal{M}_n\}$$

and set

$$\tau_k = \limsup_{n\to\infty} \tau_k(n).$$

How large is τ_k? Mohar partially answered this question by showing that for any $k \geq 2$, $\tau_k \leq \frac{1}{2}(1+\sqrt{k})$. Using the spectrum of strongly regular graphs, he also showed that

$$\tau_k \geq \frac{2\sqrt{3}}{9}\sqrt{k}\ (1+o(1)) > 0.3849\sqrt{k}\ (1+o(1)).$$

Another motivation to study these parameters is the fact that energy levels of $\pi-$electrons of hydrocarbon molecules are related to the eigenvalues of the corresponding graph and the total energy of π-electrons is related sum of the $[\frac{n}{2}]$ largest eigenvalues of their corresponding graph. In Mohar's notation, this is precisely $L_{[\frac{n}{2}]}(G)$ where G is the corresponding graph. This parameter is harder to handle analytically than $L_k(G)$ for fixed k. In Chapter 2 we will talk more about τ_k.

Similar to the question about the sum of k largest eigenvalues of graphs are the following problems:

$\max\{\lambda_1(G) + \lambda_n(G) \mid G \text{ is } K_r\text{-free}, \lvert V(G)\rvert = n\}$	Brandt [3]
$\max\{\lambda_1(G) - \lambda_n(G) \mid \lvert V(G)\rvert = n\}$	Gregory et al. [9]
$\max\{\lambda_1(G) + \lambda_n(\bar{G}) \mid \lvert V(G)\rvert = n\}$	Nosal [20], Nikiforov [18]
$\max\{\lambda_i(G) + \lambda_i(\bar{G}) \mid \lvert V(G)\rvert = n\}$	Nikiforov [19].

Results about the parameters in the left column above can be found in the references in front of them.

1.2 Some Linear Algebra

In this thesis, the acquaintance of the reader with the basic knowledge about linear algebra and graph theory is presumed.

Let $\mathbb{C}^{n\times n}$ be the set of all $n \times n$ matrices with entries from $\mathbb{C}$ and $A \in \mathbb{C}^{n\times n}$. The polynomial $\det(A - xI)$ is called the *characteristic polynomial* of A. By an *eigenvalue* of the matrix A we mean a root of its characteristic polynomial, i.e. a number $\lambda \in \mathbb{C}$ where

$$\det(A - \lambda I) = 0.$$

So, if λ is an eigenvalue of a matrix A, then $A - \lambda I$ has a nontrivial kernel. The kernel of $A - \lambda I$ is called *eigenspace* of A corresponding to the eigenvalue λ and it is a subspace of $\mathbb{C}^n$. Each nonzero vector v in the kernel of $A - \lambda I$ is called an *eigenvector* corresponding to the eigenvalue λ. Each matrix in $\mathbb{C}^{n\times n}$ has at most n eigenvalues. The *algebraic multiplicity* of an eigenvalue of a matrix is the multiplicity of it as a root of characteristic polynomial of A and the *geometric multiplicity* - or *multiplicity* - of it is the dimension of the corresponding eigenspace.

In particular, 0 is an eigenvalue of a matrix A if and only if $\det(A) = 0$. In this case, the eigenspace corresponding to the eigenvalue 0 is the kernel of A.

Example:

Let $q \in \mathbb{R}^n$. Define $A = qq^T$. Then A is a symmetric matrix, since $A^T = (qq^T)^T = qq^T = A$. Since $\operatorname{rank}(A) = 1$, $\dim(\ker(A)) = n - 1$. Therefore A has eigenvalue 0 of multiplicity

$n-1$. Moreover, we have:

$$Aq = (qq^T)q = q(q^T q) = \|q\|^2 q.$$

This shows that A has, also, eigenvalue $\|q\|^2$ with corresponding eigenvector q. So, qq^T has eigenvalue $\|q\|^2$ of multiplicity 1 and 0 of multiplicity $n-1$.

Define the inneproduct $\langle , \rangle$ on the set $\mathbb{R}^n$ by:

$$\langle x, y \rangle = x^T y.$$

In our application, we are mainly concerned with symmetric real matrices. So, let us define:

$$\mathcal{S}_n = \{A \in \mathbb{R}^{n \times n} \mid A^T = A\}$$

and

$$\mathcal{M}_n = \{A \in \mathcal{S}_n \mid 0 \leq A_{ij} \leq 1 \text{ for } 1 \leq i, j \leq n\}.$$

Theorem 1.2.1. If A is in $\mathcal{S}_n$ then all of its eigenvalues are real numbers. Also, the algebraic multiplicity of any eigenvalue of A is equal to the dimension of the corresponding eigenspace. Under the same assumption, there exists an orthogonal basis for $\mathbb{R}^n$ consisting eigenvectors of A. (See [8])

A matrix A is called *reducible* if A is similar to a block form matrix B of the form:

$$\begin{bmatrix} X & 0 \\ 0 & Y \end{bmatrix}$$

where X, Y are square matrices. If a matrix A is not reducible, we say A is an *irreducible* matrix.

We will also need the following theorem known as Perron- Frobenius theorem:

Theorem 1.2.2. Let $A = (A_{ij})$ be a non-zero $n \times n$ real irreducible symmetric matrix with non-negative entries. Then the following statements hold:

(a) There is a positive real eigenvalue λ of A such that any other eigenvalue λ' satisfies $|\lambda'| \leq \lambda$.

(b) The eigenvalue λ is a simple root of the characteristic polynomial of A. In particular, the eigenspace associated to λ is 1-dimensional.

(c) Any eigenvector corresponding to the largest eigenvalue consists of entries with the same sign and any eigenvector corresponding to the other eigenvalues, contains both positive and negative entries.

For any matrix $A \in \mathcal{S}_n$, the sequence $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ of eigenvalues of A is called the *spectrum* of A.

Theorem 1.2.3. If $A \in \mathcal{S}_n$ and $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are its eigenvalues then the eigenvalues of A^k are $\lambda_1^k, \lambda_2^k, \ldots, \lambda_n^k$.

Theorem 1.2.4. For any $A \in \mathcal{S}_n$ with the spectrum $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, we have the following identities:

$$\det(A) = \prod_{i=1}^{n} \lambda_i \quad \text{and} \quad \mathrm{tr}(A) = \sum_{i=1}^{n} A_{ii} = \sum_{i=1}^{n} \lambda_i.$$

A powerful theorem about eigenvalues of a symmetric real matrix, is a theorem known as the Courant-Fischer min-max theorem.

Theorem 1.2.5. Let $A \in \mathcal{S}_n$. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be its spectrum. Then:

$$\lambda_i = \min_{U} \max_{x \in U,\ \|x\|=1} \langle Ax, x \rangle \tag{1.1}$$

where the minimum is taken over all $(n-i+1)$-dimensional subspaces $U \subseteq \mathbb{R}^n$ (See [8]).

Of course, this theorem does not give an efficient algorithm to find the eigenvalues of A but it is useful in the theory of eigenvalues. There is also max-min version of this theorem. Proofs and extra applications of this theorem can be found, for example in [14].

1.2.1 Two Inequalities

Here, we will present two inequalities which play an important role in the next two chapters. The first inequality is the following:

Theorem 1.2.6. For any two vectors $u, v \in \mathbb{R}^n$ we have:

$$|\langle u, v \rangle|^2 \leq \|u\|^2 \|v\|^2.$$

Also, equality holds if and only if $u = cv$ for some constant $c \in \mathbb{R}$.

This theorem is known as the *Cauchy-Schwartz* inequality which holds in more general setting. For the general statement and proof one can check the book [12].

The second one is as follows:

Theorem 1.2.7. Let A, B be symmetric real matrices of order n. Let $C = A + B$. If $\lambda_n(B) \geq 0$, then $\lambda_i(A) \leq \lambda_i(C)$ for $i = 1, 2, \ldots, n$ in which $\lambda_i(X)$ is the i-th largest eigenvalue of X.

A good resource for more inequalities on matrices with the proofs is [14].

1.3 Latin Squares and Orthogonal Arrays

In this section, we will introduce *latin squares* and *orthogonal arrays*. An $n \times n$ matrix A with entries from a set S of size n (let us say $S = \{1, 2, \ldots, n\}$) is called a latin square provided that in each row and each column there is no repeated entry.

Example 1:

$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 4 & 1 & 2 & 3 \\ 3 & 4 & 1 & 2 \\ 2 & 3 & 4 & 1 \end{bmatrix} \tag{1.2}$$

Note that in this example, each row of A is obtained by a circular shift of the previous row to the right. Such a latin square is called *circulant latin square*. Apparently, if the first entry of the first row is one, then all the entries on the main diagonal of A are one. We will take advantage of this type of latin squares later.

Example 2:

Let Λ be a group of order n. Without loss of generality we can assume that the ground set of Λ is $S = \{1, 2, \ldots, n\}$. Then the multiplication table of Λ is a latin square. In fact, all the entries in the multiplication table of Λ are element of S and $a \cdot b = a \cdot c$ $(b \cdot a = c \cdot a)$ implies $b = c$. So in each row (column) there is no repeated element.

Just from the definition of latin squares, it turns out that each symbol appears exactly once in each row and each column. So, we can construct the following interesting tableau from the latin square of Example 1:

column	1 1 1 1 2 2 2 2 3 3 3 3 4 4 4 4
row	1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4
symbol	1 4 3 2 2 1 4 3 3 2 1 4 4 3 2 1

Table 1.1: A Latin square of order 4

The column $(i, j, k)^T$ in this tableau means that the symbol in the i-th column and the j-th row in the corresponding latin square is k. From the definition of latin squares, it is easy to see that if one takes any two rows of this $3 \times n^2$ tableau, each pair $(i, j) \in S \times S$ appears exactly once. This leads us to the following definition:

An *orthogonal array* with parameters n, d, denoted by $OA(n, d)$, is a tableau with n^2 columns and d rows so that each row consists of elements from the set $S = \{1, 2, \ldots, n\}$ in such a way that if way take any pair of rows, each ordered pair $(i, j) \in S \times S$ appears exactly once.

As we pointed out, any latin square gives rise to an $OA(n, 3)$. Conversely, from each $OA(n, 3)$ we can construct a latin square (and in fact more than one, since we can consider any of the rows to be the row corresponding to the rows, columns or symbols) of order n.

An interesting question about orthogonal arrays is for which values of (n, d) there exists an orthogonal array. This problem is widely open, but at least we can say that if there exists an $OA(n, d)$ then for any $1 \leq d' \leq d$ there is an $OA(n, d')$. So we can ask the following question instead:

For a given number n, what is the maximum number d so that there exists an $OA(n, d)$? This problem is still open but there are partial results on that. The following theorem is of special interest:

Theorem 1.3.1. For any positive integer n, the largest number d for which there exists an $OA(n, d)$ is at most $n+1$. Moreover, if n is a prime power then there exists an $OA(n, n+1)$.

The existence of orthogonal arrays with parameters $(n, n + 1)$ for n a prime power, is a consequence of existence of another combinatorial object called *projective plane* of these orders. In principle, the only known projective planes and orthogonal arrays with parameters $(n, n+1)$ are constructed using finite fields and since finite fields exist only for prime power , prime powers play role in this subject.

Example 3:

C1	1 1 1 1 2 2 2 2 3 3 3 3 4 4 4 4
C2	1 2 3 4 1 2 3 4 1 2 3 4 1 2 3 4
C3	1 2 3 4 2 1 4 3 3 4 1 2 4 3 2 1
C4	1 3 4 2 2 4 3 1 3 1 2 4 4 2 1 3

Table 1.2: OA(4,4)

Above is an instance of an $OA(4,4)$. The reference [23] contains a proof of Theorem 1.3.1, and more results on orthogonal arrays and latin squares.

1.4 Graphs and Eigenvalues

In this section, we will review some definitions and theorems which we will use in the next chapters. The basic knowledge of graph theory is assumed. A good reference on the basics of graph theory is [24]. The reference [8] is also a very good resource for more knowledge about some class of graphs, such as strongly regular graphs and eigenvalues of graphs.

Now we start by reviewing some needed definitions of graph theory. To any arbitrary graph, one can associate different kinds of matrices. One of the most common type of matrices associated with a given graph is its *adjacency matrix*. The adjacency matrix of a graph of order n with vertex set $\{v_1, v_2, \ldots, v_n\}$, is defined to be an n by n 01-symmetric matrix $A(G)$ where $A(G)_{ij} = 1$ if and only v_i is connected to v_j. This matrix is an element of $\mathcal{M}_n$. Notice that this definition is up to the labeling of the vertices of G. But for different labeling of G, we have different matrices which are all similar to each other. In particular, they all have the same spectrum. So the *spectrum of a graph* makes sense if we define it to be the spectrum of its adjacency matrix. In contrary, the eigenvector of a graph G makes less sense unless we specify an order on the vertex set of G. To resolve this, we define the *eigenfunction* corresponding to an eigenvalue λ of a graph G. First of all, fix a labeling $\{v_1, v_2, \ldots, v_n\}$ for the vertex set of G. Let A be the adjacency matrix of G with respect to this labeling. Let $w = (w_1, w_2, \ldots, w_n)^T$ be an eigenvector corresponding to the eigenvalue λ. Now, define eigenfunction corresponding to the eigenvalue λ to be the function:

$$f_\lambda : V(G) \to \mathbb{R} \qquad \text{where} \qquad f_\lambda(v_i) = w_i, \ i = 1, 2, \ldots, n.$$

It turns out that this definition is independent of the order of the vertices of G. In fact, we deal with adjacency matrix of a graph, as a linear operator acting on the vertex space

$\mathbb{R}^V$ where $V = V(G)$. In this setting, vectors of $\mathbb{R}^V$ are exactly the same as the functions f from V to $\mathbb{R}$. So, depending on the problem, we might use either the functional form or the matrix form of eigenvectors.

Finding the eigenvalues of a given graph is usually a hard problem but for some special cases, there are methods which help us to find the spectrum of these families. A specific example of these kind of methods, is evaluation of spectrum of *categorical product* of two graphs using the spectrum of the primal graphs. First, we define the categorical product of two graphs. If G and H are two graphs with the vertex set $V(G), W(G)$, respectively, then the *categorical product* of G and H, denoted by $G \times H$, is a graph with vertex set $V(G \times H) = V(G) \times V(H)$ and $(u, v), (u', v') \in V(G \times H)$ are adjacent if $uu' \in E(G)$ and $vv' \in E(H)$.

In Chapter 2, we will use the following theorem about eigenvalues of the categorical product of two graphs:

Theorem 1.4.1. If G and H are two graphs with spectrum $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and $\lambda'_1 \geq \lambda'_2 \geq \cdots \geq \lambda'_m$ then the eigenvalues of the graph $G \times H$ are precisely $\{\lambda_i \lambda'_j \mid 1 \leq i \leq n \text{ and } 1 \leq j \leq m\}$.

For the proof of this theorem and more examples and theorems in this matter, see [8].

One of the main importances of the adjacency matrix of a graph is to count the number of walks of specific length between two vertices. The following theorem says how we can find these numbers from the adjacency matrix of a graph.

Theorem 1.4.2. Let G be a graph with vertex set $\{v_1, v_2, \ldots, v_n\}$. If A is adjacency matrix of G with respect to this order of vertices, then the number of walks of length k from v_i to v_j is equal to A^k_{ij}.

This theorem gives an efficient algorithm for counting walks. Also we will see that there are interesting theoretical consequences of this theorem.

Clearly, the graph can be reconstructed from its adjacency matrix but in general, it can not be recovered from its spectrum (see [11]). Still the spectrum of a graph has valuable information about many parameters of the graph. In particular, there are well-known bounds on the chromatic number, clique number, independence number and more, obtained from the spectrum of the graph. There are also some other quantities, such as the number of triangles, which can be precisely determined from the spectrum.

Studying of eigenvalues of graphs and their property is part of an area in discrete mathematics known as spectral graph theory. For more on this area, one is referred to [4].

Let us mention some of the results which we will use in this thesis.

Theorem 1.4.3. For a graph G with the spectrum $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, the number of edges is given by

$$2|E(G)| = \sum_{i=1}^{n} \lambda_i^2. \tag{1.3}$$

To see the proof of this theorem, just mention that by Theorem 1.2.4 and Theorem 1.4.2 we have:

$$\sum_{i=1}^{n} \lambda_i^2 = tr(A^2) = \sum_{i=1}^{n} A_{ii}^2 = \text{number of walks of length 2 in } G = 2|E(G)|.$$

Another result which we will take advantage of, is the following theorem (see [8]):

Theorem 1.4.4. A connected graph G of order n is bipartite if and only if $\lambda_n = -\lambda_1$.

1.4.1 Strongly Regular Graphs

Now, we will investigate a class of graphs with interesting eigenvalue properties, called *strongly regular graphs*.

Let G be a k-regular graph with n vertices. In addition, suppose that

(a) Any two adjacent vertices have exactly λ common neighbors.

(b) Any two non-adjacent vertices have exactly μ common neighbors.

Then G is called a strongly regular graph with parameters (n, k, λ, μ) and denoted by $srg(n, k, \lambda, \mu)$.

Examples of srg's:

A simple example of a strongly regular graph is C_5 (i.e. the 5-cycle) which is an $srg(5, 2, 0, 1)$. Another common and less trivial example is Petersen's graph $srg(10, 3, 0, 1)$. We will exhibit larger strongly regular graphs later.

Finding strongly regular graphs is a research area with many applications in mathematical designs, coding theory and many other areas.

Let G be a graph with adjacency matrix A. The statement that G is an $srg(n, k, \lambda, \mu)$ is equivalent to the equations:

$$AJ = kJ \qquad \text{and} \qquad A^2 + (\mu - \lambda)A + (\mu - k)I = \mu J$$

where J is the $n \times n$ matrix with all entries equal to 1, and I is the identity matrix of order n.

This leads us to the important theorem below, dealing with eigenvalues of strongly regular graphs.

Theorem 1.4.5. If G is an $srg(n, k, \lambda, \mu)$ then G has eigenvalues

$$k, \frac{1}{2}\left(\lambda - \mu + \sqrt{(\mu - \lambda)^2 + 4(k - \mu)}\right) \text{ and } \frac{1}{2}\left(\lambda - \mu - \sqrt{(\mu - \lambda)^2 + 4(k - \mu)}\right)$$

of multiplicities

$$1, \frac{1}{2}\left(n - 1 + \frac{(n-1)(\mu - \lambda) - 2k}{\sqrt{(\mu - \lambda)^2 + 4(k - \mu)}}\right) \text{ and } \frac{1}{2}\left(n - 1 - \frac{(n-1)(\mu - \lambda) - 2k}{\sqrt{(\mu - \lambda)^2 + 4(k - \mu)}}\right)$$

respectively.

A non-trivial class of srg's is a family of graphs known as *Paley graphs*. These graphs are defined as follows. Let p be a prime number congruent to 1 modulo 4. It is known (see [15]) that -1 is a quadratic residue modulo p (i.e. $-1 \equiv x^2 \mod 4$ for some $x \in \mathbb{Z}_p$, finite field on p elements). Let $V(G) = \mathbb{Z}_p$ and two vertices $a, b \in V(G)$ are adjacent if and only if $a - b$ is a quadratic residue in $\mathbb{Z}_p$. As -1 is a quadratic residue, $a - b$ is residue if and only if $b - a$ is residue and therefore this definition describes an undirected graph. The graph G is called Paley graph of order p. It turns out that the Paley graph of order p is an $srg(p, \frac{p-1}{2}, \frac{p-5}{4}, \frac{p-1}{4})$.

Using the previous theorem we can easily find the spectrum of Paley graph of order p.

Theorem 1.4.6. The eigenvalues of Paley graph of order p are:

$$\frac{p-1}{2}, \frac{-1+\sqrt{p}}{2} \text{ and } \frac{-1-\sqrt{p}}{2}$$

of multiplicities

$$1, \frac{p-1}{2}, \frac{p-1}{2}$$

respectively.

In fact, we can define the Paley graph for any prime power $p \equiv 1 \pmod 4$ in the same way. The only difference is that the vertices of the graph are elements of $\mathbb{F}_p$, finite field of order p.

Another class of srg's is obtained from orthogonal arrays. Consider an orthogonal array with parameters (n, k). Construct a graph G from this array in the following way:

Assign a vertex to each column of the array and join two vertices with an edge if and only their corresponding columns have the same symbol in precisely one position. The result is an $srg(n^2, (n-1)k, n-2+(k-1)(k-2), k(k-1))$. (See [23]). In the case $k = 3$, this graph is called *latin square graph.* In Chapter 2, we will see that these graphs have large sum of eigenvalues and we can obtain "good" lower bound for τ_k from them.

Chapter 2

The Sum of k Largest Eigenvalues

In this chapter we will study the extreme behaviour of the sum of k largest eigenvalues of matrices for a given integer $k > 1$.

2.1 Upper Bound on τ_k

For a given matrix $A \in \mathcal{M}_n$ with spectrum $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ define:

$$L_k(A) := \sum_{i=1}^{k} \lambda_i$$

Mohar has introduced this parameter in [16] as a generalization of $\lambda_1 + \lambda_2$ which is studied by Gernert (see [7]) and Nikiforov (see [17]). Before we go further, we will prove two useful propositions.

Proposition 2.1.1. $\tau_{k+1} \geq \tau_k$ for any integer k.

Proof. First of all, note that if we have a graph G on n vertices with spectrum $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, then adding an isolated vertex to G adds a 0 to the spectrum of it. So $L_{k+1}(G \cup v) \geq L_k(G)$. Therefore $(n+1)\tau_{k+1}(G) \geq n\tau_k(G)$ or equivalently $\frac{n+1}{n}\tau_{k+1}(G) \geq \tau_k(G)$ for any graph G. Since this inequality holds for any graph G of n vertices, if we take the supremum of both sides with respect to G the term $\frac{n+1}{n}$ approaches to 1 and consequently, we have $\tau_{k+1} \geq \tau_k$. So, the sequence $\{\tau_k\}$ is an increasing sequence. $\square$

Proposition 2.1.2. For every integer $k \geq 1$, we have

$$\begin{aligned}\tau_k &= \sup\{\tau_k(A) \mid A \in \mathcal{M}_n \ , \ n \geq k\} \\ &= \sup\{\tau_k(A) \mid A \in \mathcal{G}_n \ , \ n \geq k\} \\ &= \limsup_{n\to\infty}\{\tau_k(A) \mid A \in \mathcal{G}_n\}\end{aligned}$$

where $\mathcal{G}_n$ is the set of adjacency matrices of all graphs on n vertices.

Proof. First, we will show that

$$\sup\{\tau_k(A) \mid A \in \mathcal{G}_n, n \geq k\} = \limsup_{n\to\infty} \{\tau_k(A) \mid A \in \mathcal{G}_n\}.$$

Consider and arbitrary graph G and let H_n be the categorical product of G and K_n for some large integer n. By Theorem 1.4.1 we can see that $\tau_k(H_n) = \frac{n-1}{n}\tau_k(G)$ and therefore,

$$\limsup_{n\to\infty} \{\tau_k(A) \mid A \in \mathcal{G}_n\} \geq \lim_{n\to\infty}(\tau_k(H_n)) = \tau_k(G).$$

Since the above inequality holds for any graph G, we can deduce that:

$$\limsup_{n\to\infty} \{\tau_k(A) \mid A \in \mathcal{G}_n\} \geq \sup\{\tau_k(A) \mid A \in \mathcal{G}_n\}.$$

On the other hand, trivially we have:

$$\limsup_{n\to\infty} \{\tau_k(A) \mid A \in \mathcal{G}_n\} \leq \sup\{\tau_k(A) \mid A \in \mathcal{G}_n\}.$$

So, we conclude that:

$$\limsup_{n\to\infty} \{\tau_k(A) \mid A \in \mathcal{G}_n\} = \sup\{\tau_k(A) \mid A \in \mathcal{G}_n\}.$$

To complete the proof of the theorem, we must show that:

$$\sup\{\tau_k(A) \mid A \in \mathcal{M}_n, n \geq k\} = \sup\{\tau_k(A) \mid A \in \mathcal{G}_n, n \geq k\}$$

Since the first supremum is taken over larger set, we can conclude that:

$$\sup\{\tau_k(A) \mid A \in \mathcal{M}_n, n \geq k\} \geq \sup\{\tau_k(A) \mid A \in \mathcal{G}_n, n \geq k\}.$$

Now, we prove the reverse inequality. Let $\varepsilon > 0$. We aim to show that

$$\sup\{\tau_k(A) \mid A \in \mathcal{M}_n, n \geq k\} \leq \sup\{\tau_k(A) \mid A \in \mathcal{G}_n, n \geq k\} + \varepsilon.$$

Take an arbitrary $A \in \mathcal{M}_n$. Since λ_i (i-th largest eigenvalue of A) is a continuous function of the entries of A, we can find a matrix $B \in \mathcal{M}_n$ with rational entries from the interval $[0,1)$ so that $L_k(A) \leq L_k(B) + \varepsilon$. Let q be the least common multiple of the denominators of the entries of B and let $N = 2nq$. Define $d_{ij} = 2qB_{ij} \in 2\mathbb{Z}$ for any $1 \leq i,j \leq n$. Let C_{ij} be a 01-symmetric matrix with exactly d_{ij} ones in each row and column and with zeros on the main diagonal. A constructive way to see the existence of such a matrix is as follows.

Take a circulant latin square of order d_{ij}. Replace any element from $\{2, 2q, 3, 2q-1, \ldots, \frac{d_{ij}}{2}+1, 2q-\frac{d_{ij}}{2}+1\}$ with 1 and any other element by 0. It can be easily observed that the way we defined the circulant latin squares guarantees that this method gives a 01-symmetric matrix with exactly d_{ij} 1s in each row and column. Moreover, since $d_{ij} = d_{ji}$, we have $C_{ij} = C_{ji}$. Now, construct an $N \times N$ block matrix X with blocks C_{ij}. From the construction of X, it is obvious that $X \in \mathcal{G}_N$.

Let λ be an eigenvalue of the matrix B with corresponding eigenvector $v = (v_1, v_2, \ldots, v_n)^T \in \mathbb{R}^n$. Let

$$w = (\underbrace{v_1, v_1, \ldots, v_1}_{2q \text{ times}}, \underbrace{v_2, v_2, \ldots, v_2}_{2q \text{ times}}, \cdots, \underbrace{v_n, v_n, \ldots, v_n}_{2q \text{ times}})^T.$$

By a simple computation we can see that

$$(Xw)_i = \sum_{j=1}^{N} X_{ij} w_j \tag{2.1}$$

$$= \sum_{j=1}^{n} d_{i'j} v_j \tag{2.2}$$

$$= \sum_{j=1}^{n} 2qB_{i'j} v_j \tag{2.3}$$

$$= 2q \sum_{j=1}^{n} B_{i'j} v_j \tag{2.4}$$

$$= 2q(Bv)_{i'} = 2q\lambda w_i \tag{2.5}$$

in which $i' \equiv i \bmod 2q$ and $1 \leq i' \leq 2q$. Therefore, X has eigenvalue $2q\lambda$ with corresponding eigenvector w. This holds for any eigenvalue λ of B so we can conclude that

$$L_k(X) \geq 2qL_k(B) \geq 2q(L_k(A) - \varepsilon)$$

or

$$\tau_k(X) \geq \tau_k(B) \geq t_k(A) - \varepsilon.$$

Since A can be any element of $\mathcal{M}_n$, we have

$$\sup\{\tau_k(A) \mid A \in \mathcal{G}_n, n \geq k\} \geq \sup\{\tau_k(A) \mid A \in \mathcal{M}_n, n \geq k\} - \varepsilon$$

and we are done. □

Proposition 2.1.2 enables us to only deal with matrices in $\mathcal{G}_n$ instead of more complicated matrices in $\mathcal{M}_n$. So, for the rest of this section, we will only deal with matrices in $\mathcal{G}_n$. So, let $A \in \mathcal{G}_n$ with spectrum $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Let G be the graph corresponding to A.

Now, we will give a lower bound on τ_k. First, we will observe that:

$$\Big(\sum_{i=1}^{k} \lambda_i\Big)^2 \leq \Big(\sum_{i=1}^{k} \lambda_i^2\Big)\Big(\sum_{i=1}^{k} 1\Big) = k\Big(\sum_{i=1}^{k} \lambda_i^2\Big) \leq 2k\|G\| \leq 2k\binom{n}{2} < kn^2$$

So if we take the square root of both sides, we will have:

$$L_k(G) = \Big(\sum_{i=1}^{k} \lambda_i\Big) \leq \sqrt{k}\, n$$

and therefore:

$$\tau_k(G) = \frac{L_k(G)}{n} < \sqrt{k}$$

for any graph G of order n. This shows that

$$\tau_k \leq \sqrt{k}$$

and the proof is completed by the previous proposition.

For $A \in \mathcal{S}_n$, we denote by $\sigma_2(A)$ the ℓ_2−norm of A,

$$\sigma_2(A) = \Big(\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}^2\Big)^{1/2}.$$

In fact, if A is adjacency matrix of a graph then $\sigma_2(A)^2$ is the number of edges of the corresponding graph.

We will present the following lemma for estimation of the eigenvalues of A in terms of $\sigma_2(A)$.

Lemma 2.1.3. If $A \in \mathcal{S}_n$ has eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$, then

$$\sum_{i=1}^{n} \lambda_i^2 = 2\big(\sigma_2(A)\big)^2.$$

Proof. By Theorem 1.2.3, we have :

$$\sum_{i=1}^{n} \lambda_i^2 = \mathrm{tr}(A^2) = \sum_{i=1}^{n} (A^2)_{ii} = \sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij}A_{ji}.$$

Since A is a symmetric matrix, we have $A_{ij} = A_{ji}$ for any $1 \le i, j \le n$ and therefore we will have:

$$\sum_{i=1}^{n} \lambda_i^2 = \sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij}^2 = 2\big(\sigma_2(A)\big)^2.$$

$\square$

Let $0 \neq q = (q_1, q_2, \dots, q_n)^T \in \mathbb{R}^n$ and $Q = qq^t$. We already saw that Q is a symmetric matrix with eigenvalues

$$\|q\|^2 > \underbrace{0 = 0 \dots = 0}_{\text{n-1 times}}$$

and q is an eigenvector of Q corresponding to the eigenvalue $\|q\|^2$. Given a matrix $A \in \mathcal{S}_n$, we define its *q-complement* as the matrix A' defined by $A' = Q - A$ where Q is as above. Let $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n$ and $\lambda'_1 \ge \lambda'_2 \ge \cdots \ge \lambda'_n$ be the spectrum of A and A', respectively.

Lemma 2.1.4. (a) $\lambda_i + \lambda'_{n-i+2} \le 0$ for $i = 2, 3, \dots, n$

(b) $\lambda_1 + \lambda'_1 \ge \|q\|^2$.

Proof. Note that part (a) is a version of Weyl inequalities. By Courant-Fischer min-max theorem we have:

$$\lambda_i = \min_{U} \max_{x \in U,\ \|x\|=1} \langle Ax, x\rangle$$

where the minimum is taken over all the subspaces of $\mathbb{R}^n$ of dimension $n - i + 1$. Let $\{y_1, y_2, \dots, y_n\}$ be an orthogonal basis for $\mathbb{R}^n$ consisting of eigenvectors of A' so that λ'_i corresponds to the eigenvalues λ'_1 for any $1 \le i \le n$. Since A' is a symmetric matrix, such a basis exists by Theorem 1.2.1. Let U_0 be the subspace generated by $\{y_1, y_2, \dots y_{n-i+2}\}$

and U_1 be the subspace generated by $\{v_{n-i+3}, v_{n-i+4}, \ldots, v_n, q\}$. Let $U_2 = U_1^{\perp}$. So, any vector in U_2 is orthogonal to all of the vectors $v_{n-i+3}, v_{n-i+4}, \ldots, v_n, q$ and in particular, to all vectors $v_{n-i+3}, v_{n-i+4}, \ldots, v_n$. Thus, U_2 is a subspace of $U_1^{\perp} = U_0$, since $\{y_1, y_2, \ldots y_n\}$ is assumed to be an orthogonal basis for $\mathbb{R}^n$. Therefore, $U_2 \subseteq U_0$. Note that U_1 is generated by $i-1$ vectors. So, $\dim(U_1) \leq i-1$ and $\dim(U_2) \geq n-i+1$. Let U' be a subspace of U_2 of dimension equal to $n-i+1$. So, U' is orthogonal to any v_i for $n \geq i \geq n-i+3$ and also to q.

Let x be an arbitrary element in U' with $\|x\| = 1$. Since $x \in U' \subseteq U_2 \subseteq U_0$,

$$x = \sum_{j=1}^{i-2} c_j v_j \qquad \text{for} \qquad c_j \in \mathbb{R}$$

and since $x \in U' \subseteq U_2 = U_1^{\perp}$, we have$\langle x, q\rangle = 0$ and therefore:

$$Qx = qq^T x = 0.$$

Now, we have:

$$\begin{aligned}
\lambda_i &= \min_{U} \max_{x \in U,\ \|x\|=1} \langle Ax, x\rangle \\
&\leq \max_{x \in U',\ \|x\|=1} \langle Ax, x\rangle \\
&= \max_{x \in U',\ \|x\|=1} \big(\langle (Q - A')x, x\rangle\big) \\
&= \max_{x \in U',\ \|x\|=1} \big(\langle Qx, x\rangle - \langle A'x, x\rangle\big) \\
&= \max_{x \in U',\ \|x\|=1} -\langle A'x, x\rangle \\
&\leq -\lambda'_{n-i+2}.
\end{aligned}$$

The last inequality holds because of the following:

$$\begin{aligned}
\langle A'x, x\rangle &= \langle A'(\sum_{j=1}^{i-2} c_j v_j), \sum_{j=1}^{i-2} c_j v_j\rangle \\
&= \langle \sum_{j=1}^{i-2} c_j \lambda'_j v_j, \sum_{j=1}^{i-2} c_j v_j\rangle \\
&= \sum_{j=1}^{i-2} c_j^2 \lambda'_j \|v_j\|^2 \\
&\geq \lambda'_{n-i+2} \sum_{j=1}^{i-2} c_j^2 \|v_j\|^2 \\
&= \lambda'_{n-i+2} \|x\|^2 \\
&= \lambda'_{n-i+2}.
\end{aligned}$$

So

$$\max_{x\in U',\ \|x\|=1} -\langle A'x, x\rangle = - \min_{x\in U',\ \|x\|=1} \langle A'x, x\rangle \leq -\lambda'_{n-i+2}.$$

For part (b), observe that $\mathrm{tr}(A)$ + $\mathrm{tr}(A')$= $\mathrm{tr}(A + A') = \mathrm{tr}(Q) = \|q\|^2$. Therefore, using the result in part (a) we have:

$$\|q\|^2 = tr(A) \ + \ tr(A') = \sum_{i=1}^{n} \lambda_i + \sum_{i=1}^{n} \lambda'_i = (\lambda_1 + \lambda'_1) + \sum_{i=2}^{n} (\lambda_i + \lambda'_i) \leq \lambda_1 + \lambda'_1.$$

□

Now we are ready to prove the main theorem of this chapter which provides a nontrivial lower bound on τ_k.

Theorem 2.1.5 (Mohar [16]). For every $k \geq 2$ we have $\tau_k \leq \frac{1}{2}(1 + \sqrt{k})$.

Proof. Note that if we can prove that $\tau_k(A) \leq \frac{1}{2}(1 + \sqrt{k})$ for any $A \in \mathcal{G}_k(n)$ then it turns out that $\sup\{\tau_k(A) \mid A \in \mathcal{G}'_n n \geq k\} \leq \frac{1}{2}(1 + \sqrt{k})$ and by Proposition 2.1.2, we can assert that $\tau_k \leq \frac{1}{2}(1 + \sqrt{k})$.

Let us take a matrix $A \in \mathcal{G}_n$. Using the above notation, define $\alpha = (\frac{1}{n}\sigma_2(A))^2$ and $\alpha' = (\frac{1}{n}\sigma_2(A'))^2$, where A' is $q-$complement of A. Here, take $q = (1, 1, \ldots, 1) \in \mathbb{R}^n$. So $Q = qq^T$ is all-1 matrix and $\|q\|^2 = n$ is the only nonzero eigenvalue of G. Notice that

$A_{ij} + A'_{ij} = Q_{ij} = 1$. So, $A'_{ij} = 1 - A_{ij}$. Using this relation and also according to the definition of $\sigma_2(A)$ and $\sigma_2(A')$, we can evaluate $\alpha + \alpha'$ as follows:

$$\begin{aligned}
\alpha + \alpha' &= (\frac{1}{n}\sigma_2(A))^2 + (\frac{1}{n}\sigma_2(A'))^2 \\
&= \frac{1}{2n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij}^2 + \frac{1}{2n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} A'^2_{ij} \\
&= \frac{1}{2n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} (A_{ij}^2 + A'^2_{ij}) \\
&= \frac{1}{2n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} (A_{ij}^2 + (1 - A_{ij})^2) \\
&= \frac{1}{2n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} (2A_{ij}^2 + 1 - 2A_{ij}) \\
&= \frac{1}{2n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} 1 \\
&= \frac{1}{2}.
\end{aligned}$$

The important fact in the above computation is that since $A \in \mathcal{G}_n$, $A_{ij} \in \{0, 1\}$ and therefore $A_{ij}^2 = A_{ij}$.

Let $\nu_i := \max\{0, \lambda_i\}$. Part (a) of Lemma 2.1.4 says that $\lambda_i \leq \lambda'_{n-i+2}$. So, by considering two cases $\lambda_i \geq 0$ or $\lambda_i < 0$ we can see that:

$$\nu_i^2 \leq \lambda'^2_{n-i+2}$$

for any $i = 2, 3, \ldots, n$. Set $t := \frac{1}{n}\lambda_1$. From the second part of the previous lemma we have:

$$\lambda'^2_1 \geq \|q\|^2 - \lambda_1 = n - \lambda_1 = n(1 - t)$$

and from it we derive that:

$$\lambda_1^2 + \lambda'^2_1 \geq t^2 n^2 + (1 - t)^2 (n)^{=} (1 - 2t(1 - t))n^2.$$

Using this inequality we have the following chain of equalities and inequalities to find an upper bound for $\sum_{i=2}^{k} \nu_i^2$:

$$
\begin{aligned}
n^2 = \frac{1}{2}2n^2 = 2n^2(\alpha + \alpha') &= 2\sigma_2^2(A) + 2\sigma_2^2(A') \\
&= \sum_{i=1}^{n} \lambda_i^2 + \sum_{i=1}^{n} \lambda_i'^2 \\
&\geq \lambda_1^2 + \lambda_1'^2 + \sum_{i=2}^{k} \lambda_i^2 + \sum_{i=2}^{k} \lambda_i'^2 \\
&\geq \lambda_1^2 + \lambda_1'^2 + \sum_{i=2}^{k} \nu_i^2 + \sum_{i=2}^{k} \lambda_i'^2 \\
&\geq \lambda_1^2 + \lambda_1'^2 + 2\sum_{i=2}^{k} \nu_i^2 \\
&\geq (1 - 2t(1-t))n^2 + 2\sum_{i=2}^{k} \nu_i^2.
\end{aligned}
$$

From above, we can deduce that:

$$
n^2 \geq (1 - 2t(1-t))n^2 + 2\sum_{i=2} k\nu_i^2.
$$

By rearrangement of the terms we have the following inequality

$$
\sum_{i=2}^{k} \nu_i^2 \leq t(1-t)n^2.
$$

In order to have an upper bound for the sum of ν_i's without square, the common trick is applying Cauchy-Schwartz inequality on the sum of squares of ν_i's. More precisely, we have:

$$
\begin{aligned}
\Big(\sum_{i=2}^{k} \nu_i\Big)^2 &\leq \Big(\sum_{i=2}^{k} 1\Big)\Big(\sum_{i=2}^{k} \nu_i^2\Big) \\
&\leq (k-1)\Big(\sum_{i=2}^{k} \nu_i\Big)^2 \\
&\leq (k-1)t(1-t)n^2
\end{aligned}
$$

or

$$
\sum_{i=2}^{k} \nu_i \leq n\sqrt{(k-1)t(1-t)}.
$$

From the definition of ν_i we can see that $\nu_i \geq \lambda_i$. So, the above upper bound gives rise to an upper bound for sum of $\lambda_2, \lambda_3, \dots \lambda_k$. Also mention that $\lambda_1 = nt$ so it turns out that

$$\tau_k(A) = \frac{1}{n}\sum_{i=1}^{k} \lambda_i \leq \frac{1}{n}(nt + n\sqrt{(k-1)t(1-t)}) = t + \sqrt{(k-1)t(1-t)}$$

In order to get rid of t in the previous upper bound on $\tau_k(A)$, we can maximize the function $f(t) = t + \sqrt{(k-1)t(1-t)}$ for a fixed k. Since t is defined to be the ratio of λ_1 and n and $\lambda_1 \leq n-1$, $t \in [0,1)$. We can see that $f'(t) = 1 + \sqrt{k-1}\frac{1-2t}{2\sqrt{t-t^2}}$. If we equate $f'(t) = 0$ and solve it for t, it follows that f has an optimum value at the point $t = \frac{1}{2}(1 + k^{-1/2})$. Also by taking the second derivative of f it turns out that this point is a maximum point for the function and the maximum value of f is going to be $\frac{1}{2}(1+\sqrt{k})$. So, we will have:

$$\tau_k(A) \leq \frac{1}{2}(1+\sqrt{k})$$

and therefrom we get, $\tau_k \leq \frac{1}{2}(1+\sqrt{k})$. This completes the proof of the theorem. □

Corollary 2.1.6. If $a < b$ are two real numbers and n is an integer number, then for any matrix $A \in \mathcal{S}_n$ whose entries are between a and b, and for any $2 \leq k \leq n$, we have:

$$\frac{\lambda_1 + \lambda_2 + \ldots + \lambda_k}{n} = \frac{L_k(A)}{n} = \tau_k(A) \leq \frac{b-a}{2}(1+\sqrt{k}) + \max\{0, a\}.$$

Proof. Let Q be the all-1-matrix and consider the matrix $B = A - aQ$ and $C = \frac{1}{b-a}B$. Since the entries of A are between a and b, the entries of B are between 0 and $b-a$ and entries of C are between 0 and 1. Also, since, both A and Q are matrices in $\mathcal{S}_n$, we can say that $C \in S_n$ and therefore, $C \in \mathcal{M}_n$. Now we can apply Theorem 2.1.5 and conclude that $\tau_k(C) \leq \tau_k \leq \frac{1}{2}(1+\sqrt{k})$.

Also, from the definition of C, we have $\lambda_i(B) = (b-a)\lambda_i(C)$ where λ_i denotes the i-th largest eigenvalue. So, we have:

$$L_k(B) = (b-a)L_k(C) \leq (b-a)n\tau_k \leq (b-a)\frac{n}{2}(1+\sqrt{k}).$$

Since the eigenvalues of the matrix Q are all non-negative real numbers and $A = B + aQ$, by Theorem 1.2.7 we can assert that:

$$\lambda_i(A) \leq \lambda_i(B) + \lambda_i(aQ)$$

and therefore:

$$\begin{aligned}\sum_{i=1}^{k}\lambda_i(A) &\leq \sum_{i=1}^{k}\lambda_i(B)+\sum_{i=1}^{k}\lambda_i(aQ)\\ &\leq \frac{n}{2}(b-a)(1+\sqrt{k})+\sum_{i=1}^{k}\lambda_i(aQ)\\ &\leq \frac{n}{2}(b-a)(1+\sqrt{k})+\max\{0,a\}n.\end{aligned}$$

The last inequality is because the eigenvalues of aQ are from $\{an, 0\}$. So, the sum of k largest eigenvalues of aQ, which is the same as $L_k(aQ)$, equals $\max\{0, a\}n$. Thus:

$$\sum_{i=1}^{k}\lambda_i(A) \leq \frac{n}{2}(b-a)(1+\sqrt{k})+\max\{0,a\}n. \tag{2.6}$$

Now, if we divide both sides of Equation 2.6 by n, we will have:

$$\tau_k(A) \leq \frac{b-a}{2}(1+\sqrt{k})+\max\{0,a\}.$$

□

2.2 Lower Bound on τ_k

In the previous section, we showed that $\tau_k(A) \leq \frac{1}{2}(1+\sqrt{k})$. Our strategy was comparing the eigenvalues of the complementary matrix. Then, we derived an upper bound for the sum of squares of k largest eigenvalues of the matrix and finally using the Cauchy-Schwartz inequality, we got an upper bound for the sum of k largest eigenvalues of the matrix. Therefore, roughly speaking, in order to have a matrix $A \in \mathcal{G}_n$ with $L_k(A)$ close to $\frac{1}{2}(1+\sqrt{k})n$, it makes sense to check the matrices in $\mathcal{G}_n$ with all the inequalities we used in the proof of Theorem 2.1.5, are close to be equalities.

In other words, a natural way to find a matrix $A \in \mathcal{G}_n$ with extreme $L_k(A)$ is a matrix with these rough properties:

- Both A and its complementary matrix A' must have $\Theta(n^2)$ 1's.
- Almost all of the k largest eigenvalues of A must be close to each other.

So, if the k largest eigenvalues of A are close to each other and they sum to $c(1+\sqrt{k})n$ for some constant c close to $\frac{1}{2}$, then they must be approximately $cnk^{-1/2}$.

This "*extreme*" behavior is exhibited in some well-known families of graphs. We will investigate the behavior of $L_k(A)$ when A is adjacency matrix of a graph in either of these families.

2.2.1 τ_k of Paley Graphs

The first family of graphs which we will consider are Paley graphs P_n where $n \equiv 1 \mod 4$ is a prime number. Let A to be the adjacency matrix of P_n and $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the spectrum of A. Let $k = \frac{n-1}{2}$. By Theorem 1.4.6, we have $\lambda_1 = \frac{n-1}{2}$ and $\lambda_i = \frac{1}{2}(\sqrt{n}-1)$ for $i = 2, 3, \ldots, k$. So, we have:

$$\tau_k(A) = \frac{n-1}{2} + \frac{1}{2}(\sqrt{n}-1)(k-1)$$

Since $k = \frac{n-1}{2}$, we have:

$$\tau_k \geq \tau_k(A) = \frac{2k}{4k+2} + \frac{k-1}{4k+2}(\sqrt{2k+1}-1) = \frac{1}{4}(\sqrt{2k+1}+1) + o(1).$$

and therefrom, we get:

$$\tau_k \geq \frac{1}{4}(\sqrt{2k+1}+1)$$

provided that $n = 2k+1 \equiv 1 \pmod 4$ is a prime number.

Now, the question is that, how about the other k's which are not of this form. The point is that, a strong theorem about distribution of prime numbers implies that for any $\varepsilon > 0$ there exist a sufficiently large number N so that for any $k \geq N$ there is a prime number $p \equiv 1 \mod 4$ between $(1-\varepsilon)k$ and k (see [1]). So, for a fixed $\varepsilon > 0$ and a given k we can find a prime number $p \equiv 1 \mod 4$ so that $2(1-\varepsilon)k + 1 \leq p \leq 2k+1$ provided that k is large enough. Let $k' = \frac{p-1}{2}$ or equivalently $p = 2k'+1$. So, $2(1-\varepsilon)k+1 \leq 2k'+1 \leq 2k+1$ or $(1-\varepsilon)k \leq k' \leq k$.

By Proposition 2.1.1, we know that τ_k is an increasing function of k. Thus, we can assert that $\tau_k \geq \tau'_k$. Since $2k'+1 = p \equiv 1 \mod 4$, the above argument implies that:

$$\tau'_k \geq \frac{1}{4}(\sqrt{2k'+1}+1) \geq \frac{1}{4}(\sqrt{2(1-\varepsilon)k+1}+1).$$

Finally we have:

$$\tau_k \geq \frac{1}{4}\big(\sqrt{2(1-\varepsilon)k+1}+1\big).$$

Since ε is any arbitrary positive number, the following theorem follows:

Theorem 2.2.1 (Mohar [16]). For any k, $\tau_k \geq \frac{1}{4}\sqrt{2k+1}(1+o(1)) > 0.35355(\sqrt{k}+1)\big(1+o(1)\big)$.

2.2.2 τ_k of Orthogonal Array Graphs

Another class of graphs with the similar behavior of the eigenvalues is the class of graphs of orthogonal arrays which were introduced in the first chapter.

Recall that to an $OA(N,d)$ we can assign an $srg(N^2, k(N-1), N-2+(d-1)(d-2), d(d-1)$ with eigenvalues

$$\begin{aligned}
&k(N-1),\\
&\frac{1}{2}\big(N-2+(d-1)(d-2)-d(d-1)+\\
&\sqrt{(d(d-1)-(N-2+(d-1)(d-2)))^2+4(d(N-1)-d(d-1))}\big),\\
&\frac{1}{2}\big(N-2+(d-1)(d-2)-d(d-1)-\\
&\sqrt{(d(d-1)-(N-2+(d-1)(d-2)))^2+4(k(N-1)-d(d-1))}\big)
\end{aligned}$$

with multiplicities

$$\begin{aligned}
&1,\\
&\frac{1}{2}\Big(N^2-1+\frac{(N^2-1)(d(d-1)-(N-2+(d-1)(d-2)))-2d(N-1)}{\sqrt{(d(d-1)-(N-2+(d-1)(d-2)))^2+4(d(N-1)-d(d-1))}}\Big)\\
&\frac{1}{2}\Big(N^2-1-\frac{(N^2-1)(d(d-1)-(N-2+(d-1)(d-2)))-2d(N-1)}{\sqrt{(d(d-1)-(N-2+(d-1)(d-2)))^2+4(d(N-1)-d(d-1))}}\Big)
\end{aligned}$$

respectively.

The "extremal" behaviour with respect to τ_k in this family of graphs is achieved for $d \approx \frac{1}{3}N$ where it gives the bound

$$\tau_k \geq \frac{2\sqrt{3}}{9}\sqrt{k} > 0.3849\sqrt{k}$$

for $k = d(N-1)$. Notice that this bound only holds if we have an $OA(N,d)$ where $d \approx \frac{1}{3}N$. The only known such orthogonal arrays are those where N is a prime power.

The similar strategy as we did in the previous section shows that this bound can be generalized for any k if we add a factor $1 + o(1)$. So we have the following theorem:

Theorem 2.2.2 (Mohar [16]). For any integer $k > 1$ we have:

$$\tau_k \geq \frac{2\sqrt{3}}{9}\sqrt{k}(1+o(1)) > 0.3849\sqrt{k}(1+o(1)).$$

2.2.3 τ_k of Some Strongly Regular Graphs

Consider a graph $G = srg(n, d, \lambda, \mu)$ for appropriate parameters n, d, λ, μ. As we saw in Theorem 1.4.5, G has only three eigenvalues. One of them is d of multiplicity 1 and there are two more. One is positive and the other is negative. If we let k be the number of positive eigenvalues of G then we can compute $\tau_k(G)$ using Theorem 1.4.5, as a lower bound for τ_k. There is a list of admissible parameters of strongly regular graphs up to 1000 vertices by Gordon Royle [21] which we can take advantage of.

The bound which we get this way is very close to the upper bound we have. (recall that we showed $\tau_k/(\sqrt{k}+1) \leq 1/2$)

Table 2.1 is obtained by examining some of strongly regular graphs from Royle's list.

srg parameters	k	$\tau_k(G)/(\sqrt{k}+1)$
(736,364,204,156)	47	0.4766713
(800,376,204,152)	48	0.4742562
(931,450,241,195)	76	0.4725182
(540,266,148,114)	46	0.4702009
(784,348,182,132)	49	0.4687500
(276,135,78,54)	24	0.4643397

Table 2.1: $\tau_k(G)/(\sqrt{k}+1)$ for some srg's

2.2.4 Taylor Graphs

Another class of strongly regular graphs is Taylor graphs (see [22]). In our application, we need a family of Taylor graphs which is obtain as follows.

Let q be an odd prime power and let H be a non-degenerate Hermitian form in the projective geometry $PG(2,q^2)$. Let U be the corresponding Hermitian curve. So we have $|U| = q^3+1$. Let Δ be the set of all triples $\{x,y,z\}$ from U such that $H(x,y)H(y,z)H(y,z)$ is a quadratic residue in the field $GF(q^2)$ if $q \equiv 3 \mod 4$ and is a quadratic non-residue in $GF(q^2)$ if $q \equiv 1 \mod 4$. Taylor has proved (see [22]) that there is a graph G with the vertex set U such that the triples $\{x,y,z\}$ of vertices is in Δ if and only if the subgraph induced by these three vertices has either one or three edges. Moreover, for every $u \in U$ there is a unique such a graph for which the vertex u has degree 0. We will call this graph G_u. Let H'_u be the graph obtained by deleting the vertex u from G_u. Taylor proved that H'_u is a strongly regular graph. Thus the complement of it is also an srg. We call the complement of H'_u, H_u. It turns out that the parameters of srg H_u is $\left(q^3, \frac{1}{2}(q+1)(q^2-1), \frac{1}{4}(q+3)(q^2-3)+1, \frac{1}{4}(q+1)(q^2-1)\right)$. Then we can find the eigenvalues of H_v. The largest eigenvalue of H_u is $\lambda_1 = \frac{1}{2}(q+1)(q^2-1)$ with multiplicity one. the second largest is $\lambda_2 = \frac{1}{2}(q^2-1)$ with multiplicity $q(q-1)$. So if we let $k = q(q-1)+1$ then we have:

$$\tau_k(H_u) = \frac{1}{2q^3}\left((q+1)(q^2-1) + q(q-1)(q^2-1)\right) = \frac{q^4-1}{2q^3}.$$

A routine computation shows that we have:

$$\tau_k \geq (\sqrt{k}+1)(\frac{1}{2} - \frac{1}{4}k^{-1/2} + \frac{1}{16}k^{-3/2} + O(k^{-2})).$$

Note that this bound is valid only if k is of the form q^2-q+1 where q is an odd prime power. By the same strategy as before, we can extend our result for any constant k to get the following result:

Theorem 2.2.3 (Mohar [16]). $\tau_k \geq (\sqrt{k}+1)(\frac{1}{2} - \frac{1}{4}k^{-1/2} - o(k^{-9/10}))$.

2.2.5 τ_k of Random Graphs

Random graphs $\mathcal{G}(n,1/2)$ is another interesting family of graphs with similar behavior of the eigenvalues as Paley graphs. So, in this section we will study the bound for τ_k obtained from random graphs. From a result by Füredi and Komlós (see [6]), the largest eigenvalue of random graphs $\mathcal{G}(n,1/2)$ is close to $\frac{n}{2}$ with high probability and all other eigenvalues almost surely have absolute value $O(\sqrt{n})$. This means a random graph from $\mathcal{G}(n,1/2)$ has the property that except the largest eigenvalue, all its other $k-1$ largest eigenvalues close to each other if k is a fixed number. This property is one of the properties that we expect a graph with extreme sum of k largest eigenvalues should have. So, another family of candidates of graphs to give a good lower bound on τ_k is the family of random graphs. We might consider other models of randomness which gives the better results but at least, among the families of the form $\mathcal{G}(n,p)$, the best choice is $p = 1/2$. In fact, as we saw before, graphs with extreme behaviour of sum of k largest eigenvalues are expected to have about half of the possible edges. This shows that the best choice of p is $p = 1/2$.

Another result in that regard appears in a paper by Wigner (see [25]) who gives the density of eigenvalues distribution of random graphs. This result, known as Wigner's semicircle law, shows that the number of eigenvalues that are greater than $\sqrt{2nt}$ is approximately equal to

$$k = k_n(t) = \frac{2n}{\pi}\int_t^1 \sqrt{1-x^2}dx = \frac{n}{2\pi}(2t\sqrt{1-t^2} - 2\arcsin(t) + \pi)$$

and the sum of these eigenvalues is approximately:

$$s_n(t) = \frac{2n^{3/2}}{\pi}\int_t^1 x\sqrt{1-x^2}dx = \frac{2n^{3/2}}{3\pi}(1-t^2)^{3/2}.$$

By using the value $t = 0.293435$ (which seems to give almost best possible result according to computational experiments), we obtain the following lower bound:

$$\tau_k \geq \tau_k(n) \geq \frac{s_n(t)}{n}(1+o(1)) > 0.32985\sqrt{k}(1+o(1)).$$

Chapter 3

Sum Of The Two Largest Eigenvalues of Graphs

3.1 Matrices with constant row sums

Assume that $A \in \mathcal{M}_n$ is a matrix with constant row sums, i.e.,

$$\sum_{j=1}^{n} A_{ij} = r \qquad i = 1, \ldots, n$$

holds for some constant r $(0 \leq r \leq n)$. As an example, the adjacency matrix of any r-regular graph of order n is such a matrix.

Define $\bar{A} \in \mathcal{M}_n$ to be the matrix with $\bar{A}_{ij} = 1 - A_{ij}$, i.e., $\bar{A} = J - A$, where J is the all-1-matrix of order n. Let $\mathbf{j} = (1, 1, \ldots, 1)^T \in \mathbb{R}^n$. We have:

$$(A\mathbf{j})_i = \sum_{k=1}^{n} A_j k \cdot 1 = r$$

and therefore:

$$(A\mathbf{j}) = r\mathbf{j}.$$

Moreover, as we saw in the first chapter, $\mathbf{j}$ is an eigenvector of the matrix $J = \mathbf{j}\mathbf{j}^T$ corresponding to the eigenvalue $\|\mathbf{j}\|^2 = n$.

Now we can see that $\mathbf{j}$ is an eigenvector of $\bar{A}$ corresponding to the eigenvalue $n - r$ since we have:

$$\bar{A}\mathbf{j} = (J - A)\mathbf{j} = n\mathbf{j} - r\mathbf{j} = (n - r)\mathbf{j}.$$

So, $\mathbf{j}$ is an eigenvector for both matrices, A and $\bar{A}$, corresponding to the eigenvalues r and $n-r$, respectively. Furthermore, by the Perron-Frobenius theorem, these are the largest eigenvalues of these two matrices since they only contain positive entries.

As we pointed out earlier, since A is symmetric, there is an orthogonal basis $\mathcal{B}$ for $\mathbb{R}^n$ consisting of eigenvectors of A. Without loss of generality, we can assume that $\mathcal{B}$ contains $\mathbf{j}$.

Suppose that u is another element of $\mathcal{B}$. Since u is orthogonal to $\mathbf{j}$ and $J = \mathbf{j}\mathbf{j}^T$, we have:

$$Au + \bar{A}u = Ju = \mathbf{j}\mathbf{j}^T u = 0.$$

This implies that $Au = -\bar{A}u$. The same argument works if we interchange the role of A and $\bar{A}$. In particular, if we take u to be an eigenvector corresponding to the second largest eigenvalue of A, then $\bar{A}u = -Au = \lambda_2 u$ where λ_2 is the second largest eigenvalue of A. Hence, the negative of the second largest eigenvalue of A is an eigenvalue of $\bar{A}$. Thus we have $-\lambda_2 \geq \bar{\lambda_n}$ where $\bar{\lambda_n}$ is the smallest eigenvalue of $\bar{A}$. On the other hand, by Perron-Frobenius Theorem, $|\bar{\lambda_n}| \leq \bar{\lambda_1} = n-r$. Hence, $\lambda_2 \leq -\bar{\lambda_n} \leq \bar{\lambda_1} = n-r$ or simply $\lambda_2 \leq n-r$. Consequently:

$$\tau_2(A) \leq \tfrac{1}{n}(r + (n-r)) = 1.$$

This proves the following proposition:

Proposition 3.1.1. If $A \in \mathcal{M}_n$ has constant row sums, then $\tau_2(A) \leq 1$.

Corollary 3.1.2. If G is a regular graph of order n, then the sum of two largest eigenvalues of G is at most $n-2$.

Proof. Apply the previous proposition to the matrix $A^+ = A + I$ where A is the adjacency matrix of G and I is identity matrix of size n. So we will have $\lambda_1(A^+) + \lambda_2(A^+) \leq n$ where $\lambda_1(A^+) \geq \lambda_2(A^+)$ are two largest eigenvalues of A^+. So by definition of A^+ we have

$$\lambda_1(A) + \lambda_2(A) = \lambda_1(A^+) + \lambda_2(A^+) - 2 \leq n - 2.$$

□

3.2 Graphs with extreme eigenvalue sum

In this section we will present a family of graphs on $7n$ vertices with $\lambda_1 + \lambda_2 = 8n - 2$. We believe that these graphs are extreme examples for the value of τ_2.

Before we go further, we need the following lemma about the eigenvalues and eigenfunctions of graphs:

Lemma 3.2.1. Let G be a graph with vertex set $V = \{v_1, v_2, \ldots, v_n\}$. Let A be the adjacency matrix of G with respect to the order $v_1, v_2, \ldots, v_n$. If λ is an eigenvalue of A and $f : V \to \mathbb{R}$ is a corresponding eigenfunction, then we have:

$$\lambda f_i = \sum_{v_i v_j \in E(G)} f_j$$

in which $f_i = f(v_i)$.

Proof. Consider the vector form of the theorem. If we take $x = (f_1, f_2, \ldots, f_n)$ then x is an eigenvector of A corresponding to the eigenvalue λ so we have $Ax = \lambda x$. Now, let us compute the $i - th$ coordinate of both sides of this equation. The $i - th$ coordinate of the right hand side is obviously λf_i. For the left hand side we have:

$$(Ax)_i = \sum_{j=1}^{n} A_{ij} f_j.$$

Note that any A_{ij} is either 0 or 1. The 0 terms does not affect the summation and also $A_{ij} = 1$ iff $v_i v_j \in E(G)$. So we can rewrite the above equation as

$$(Ax)_i = \sum_{v_i v_j \in E(G)} f_j.$$

Therefore,

$$\lambda f_i = \sum_{v_i v_j \in E(G)} f_j.$$

□

If G is a graph and $v \in V(G)$, we denote by $N[v]$ the set of the neighbors of v together with v, and call it the *closed neighborhood* of v. We will use the following lemma to find the spectrum of graphs with many vertices whose closed neighborhoods are the same.

Lemma 3.2.2. Suppose that G is a simple graph and u, v are vertices of G such that $N[u] = N[v]$. If $\lambda \neq -1$ is an eigenvalue of G and $f : V(G) \to \mathbb{R}$ is a corresponding eigenfunction, then $f(u) = f(v)$.

Proof. Since f is an eigenfunction corresponding to the eigenvalue λ, by the previous lemma we have:

$$\sum_{x \in N[u] \setminus \{u\}} f(x) = \lambda f(u) \qquad \text{and} \qquad \sum_{x \in N[v] \setminus \{v\}} f(x) = \lambda f(v).$$

Since $N[u] = N[v]$, these two equations imply that

$$\lambda f(u) + f(u) = \sum_{x \in N[u]} f(x) = \sum_{x \in N[v]} f(x) = \lambda f(v) + f(v).$$

This implies that $(\lambda + 1)(f(u) - f(v)) = 0$. Since $\lambda \neq -1$, we conclude that $f(u) = f(v)$. $\square$

Let $n \geq 1$ be an integer. Let $G_n = K_{7n} - E(K_{2n,2n})$ be the graph on $7n$ vertices, which is obtained from the complete graph on vertex set $V = X \cup Y \cup Z$ with $|X| = 3n$ and $|Y| = |Z| = 2n$ by removing all edges between Y and Z. We will show that the sum of two largest eigenvalues of G_n is $8n - 2$.

Theorem 3.2.3. The eigenvalues of the graph G_n, defined above, are $\lambda_1 = 6n - 1$, $\lambda_2 = 2n - 1$, $\lambda_{7n} = -n - 1$, and $\lambda_i = -1$ for $i = 3, 4, \ldots, 7n - 1$. In particular, $\lambda_1 + \lambda_2 = 8n - 2$.

Proof. Let $\lambda \neq -1$ be an eigenvalue of G and $f : V \to \mathbb{R}$ be a corresponding eigenfunction. Since all vertices in each of the three parts X, Y, Z have the same closed neighborhoods, f takes the same value in each part by Lemma 3.2.2. So assume that $f(v) = x$ for $v \in X$, $f(v) = y$ for $v \in Y$, and $f(v) = z$ for $v \in Z$.

It is convenient to look at f as an eigenfunction of the matrix $B = A(G) + I$ for the eigenvalue $\mu = \lambda + 1 \neq 0$. As μ is an eigenvalue, by Lemma 3.2.1 we have the following three characteristic equations:

$$\mu x = 2nx + 3ny \tag{3.1}$$

$$\mu y = 2nx + 3ny + 2nz \tag{3.2}$$

$$\mu z = 3ny + 2nz. \tag{3.3}$$

After dividing by n, the system (3.1)–(3.4) is changed to

$$tx = 2x + 3y \tag{3.4}$$

$$ty = 2x + 3y + 2z \tag{3.5}$$

$$tz = 3y + 2z \tag{3.6}$$

where $t = \mu/n$. This is a system of linear equations which can also be written as $(x, y, z)(C - tI) = 0$ where

$$C = \begin{bmatrix} 2 & 2 & 0 \\ 3 & 3 & 3 \\ 0 & 2 & 2 \end{bmatrix}.$$

The nontrivial solutions correspond to the eigenvalues $t = 6$, $t = 2$, and $t = -1$ of the matrix C, yielding three solutions, $6n$, $2n$, and $-n$, for μ. This gives three solutions $6n - 1$, $2n - 1$, and $-n - 1$ for $\lambda = \mu - 1$, as claimed. □

Corollary 3.2.4. $\tau_2 \geq \frac{8}{7} > 1.14285$.

Proof. Theorem 3.2.3 shows that $\tau_k(n) \geq \frac{8}{7} - \frac{2}{n}$. So, if n approaches to infinity, it turns out that $\tau_2 \geq \frac{8}{7}$ □

So far, it is the best lower bound on τ_2

3.3 Upper bounds

In this section, we aim to exhibit Nikiforov's upper bound on τ_2. Namely:

Theorem 3.3.1 (Nikiforov [17]). $\tau_2 \leq \frac{2}{\sqrt{3}}$.

Let $A \in \mathcal{M}_n$, and $\sigma_2(A)$ to be the ℓ_2-norm of A defined in the previous chapter. We shall need an estimate on the eigenvalues of A in terms of $\sigma_2(A)$. For a symmetric matrix $A \in \mathbb{R}^{n\times n}$ we define the *graph of A* as the graph $G(A)$ with vertex set $\{1, \ldots, n\}$ in which two vertices are adjacent if and only if $A_{ij} \neq 0$. Notice that $G(A)$ has loops if A has some nonzero diagonal entries.

Lemma 3.3.2. If $A \in \mathcal{M}_n$, then

(a) $\lambda_1^2 + \lambda_2^2 + \cdots + \lambda_n^2 = 2\big(\sigma_2(A)\big)^2$, and

(b) $|\lambda_n| \leq \sigma_2(A)$, where the equality holds if and only if the graph of A is bipartite and $\text{rank}(A) \leq 2$.

Proof. Since $A \in \mathcal{M}_n$, A is a symmetric matrix and $A_{ij} = A_{ji}$ so,

$$(A^2)_{ii} = \sum_{j=1}^{n} A_{ij}A_{ji} = \sum_{j=1}^{n} A_{ij}^2.$$

Therefore we have:

$$2\sigma_2(A)^2 = \text{tr}(A^2) = \sum_{i=1}^{n} \lambda_i^2. \tag{3.7}$$

This proves (a).

Now, notice that by Perron-Frobenius Theorem, $|\lambda_n| \leq \lambda_1$. Therefore by applying the result from part (a) we have:

$$\lambda_n^2 \leq \frac{1}{2}(\lambda_1^2 + \lambda_n^2) \leq \frac{1}{2}(\lambda_1^2 + \lambda_2^2 + \cdots + \lambda_n^2) = \sigma_2^2. \tag{3.8}$$

Observe that the equality holds in (3.8) if and only if $\lambda_2 = \lambda_{n-1} = 0$, i.e., when $\lambda_2 = 0$ and $\text{rank}(A) \leq 2$. By the Perron-Frobenius Theorem, $\lambda_1 \geq |\lambda_n|$, with equality if and only if the graph of A is bipartite. This is because $\lambda_2 = 0$ implies that the graph is connected up to possible isolated vertices. Thus,

$$2\sigma_2(A)^2 \geq \lambda_1^2 + \lambda_n^2 \geq 2\lambda_n^2$$

with equality if and only if the graph of A is bipartite, $\text{rank}(A) \leq 2$, and $\lambda_2 = 0$.

To conclude the proof, we have to show that the first two conditions ($G(A)$ is bipartite and $\text{rank}(A) \leq 2$) imply that $\lambda_2 = 0$. Let x be the Perron-Frobenius eigenvector for the eigenvalue λ_1 of A. Let $V(G(A)) = U \cup W$ be a bipartition of the graph of A, and let y be the vector whose values are $y_v = x_v$ if $v \in U$ and $y_v = -x_v$ if $v \in W$. Then we claim that $Ay = -\lambda_1 y$. We can pretend that rows and columns of A are labeled with vertices of its graph G. Let $v \in W$ be an arbitrary vertex of G. Now, we will compute $(Ay)_v$. We have:

$$(Ay)_v = \sum_{u \in V(G)} A_{vu} y_u.$$

Since $v \in W$ therefore by our assumption $A_{vu} = 0$ for every $u \in W$. Also, if $u \in U$ then $y_u = x_u$. Thus the previous equation can also be written as :

$$(Ay)_v = \sum_{u \in V(G)} A_{vu} y_u = \sum_{u \in V(G)} A_{vu} x_u = (Ax)_v = \lambda_1 x_v = -\lambda_1 y_v.$$

Similarly, we can show that $(Ay)_u = -\lambda_1 y_u$ for $u \in U$. This proves the claim.

If $A \neq 0$, A has two non-zero eigenvalues λ_1 and $-\lambda_1$. If the rank of A is at most two, this implies that $\dim(\ker(A)) = n-2$. Thus A has eigenvalue zero of multiplicity $n-2$. This means all other eigenvalues are zero. This completes the proof. □

Given a matrix $A \in \mathcal{M}_n$, let A' be its "complement", defined by $A' = J - A$, where J is the all-1 matrix of order n. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of A in the decreasing order, and let $\lambda'_1 \geq \lambda'_2 \geq \cdots \geq \lambda'_n$ be the eigenvalues of A'.

A theorem of Weyl (see [14, Theorem 4.3.1]) relates eigenvalues of two matrices $A, B \in \mathbb{R}^n$ and the eigenvalues of their sum $A + B$:

$$\lambda_i(A) + \lambda_n(B) \leq \lambda_i(A+B), \qquad 1 \leq i \leq n. \tag{3.9}$$

In the special case of complementary matrices A and A', their sum $J = A + A'$ has one simple eigenvalue equal to n, and all other eigenvalues are zero. The Weyl inequality (3.9) for $i = 2$ then yields:

Lemma 3.3.3. $\lambda_2 \leq |\lambda'_n|$.

We are now ready for the proof of Theorem 3.3.1. Let us define

$$\begin{aligned} t &= (\lambda_1 + \cdots + \lambda_k)/n, \\ \alpha &= (\sigma_2(A)/n)^2, \\ \alpha' &= (\sigma_2(A')/n)^2, \\ \beta' &= \sqrt{\alpha'}. \end{aligned}$$

Let us observe that

$$\begin{aligned} \alpha + \alpha' &= \frac{1}{2n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}(a_{ij}^2 + (1-a_{ij})^2) \\ &= \frac{1}{2n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}(1 + 2a_{ij}^2 - 2a_{ij}) \qquad (3.10) \\ &= \frac{1}{2} - (\sigma_1(A) - \sigma_2(A)^2)n^{-2}. \qquad (3.11) \end{aligned}$$

Since $0 \leq a_{ij} \leq 1$, we have $a_{ij}^2 + (1-a_{ij})^2 \geq \frac{1}{2}$. Thus, (3.10) and (3.11) yield the following bounds on $\alpha + \alpha'$:

$$\frac{1}{4} \leq \alpha + \alpha' \leq \frac{1}{2}. \tag{3.12}$$

Lemmas 3.3.2 and 3.3.3 imply that

$$\lambda_2 \leq |\lambda'_n| \leq \beta' n.$$

By combining the above inequalities, we get:

$$\begin{aligned}\lambda_1^2 + 3\lambda_2^2 &\leq \lambda_1^2 + \lambda_2^2 + 2\lambda_2'^2 \\ &\leq \lambda_1^2 + \lambda_2^2 + \lambda_1'^2 + \lambda_2'^2 \\ &\leq 2(\alpha + \alpha')n^2 \leq n^2.\end{aligned}$$

This implies that

$$(\lambda_1 + \lambda_2)^2 \leq (1 + \frac{1}{3})(\lambda_1^2 + 3\lambda_2^2) \leq \frac{4}{3} n^2$$

which in turn implies the inequality $\lambda_1 + \lambda_2 \leq \frac{2}{\sqrt{3}} n$ proved by Nikiforov in [17].

3.4 The sum of three largest eigenvalues of graphs

In this section, we will present an upper bound for τ_3. Recall that in Chapter 2 we showed that for any $k \geq 2$ we have $t_k \leq \frac{1}{2}(\sqrt{k} + 1)$. Note that this is a general bound for any value of k but for specific k we may find better upper bounds, as we did in the previous chapter for $k = 2$. For $k = 3$ we have the following new result:

Theorem 3.4.1. $\tau_3 \leq \frac{3}{\sqrt{5}} < 1.3417$.

Proof. As we showed in Proposition 2.1.2, in order to prove the theorem, it suffices to show that for any graph G, $\tau_3(G) \leq \frac{3}{\sqrt{5}}$. So, Let G be an arbitrary graph with n vertices and m edges. Let $l_1 \geq l_2 \geq \lambda_3$ be three largest eigenvalues of G and $\mu_n \leq \mu_{n-1}$ be two smallest eigenvalues of $\bar{G}$, the complement of G.

If $\lambda_3 \leq 0$ then $L_3(G) \leq L_2(G) \leq n\tau_2(G) < 1.3n$ and we are done. Otherwise, $\lambda_3 > 0$.

By Weyl inequalities we have:

$$\lambda_2 + \mu_n \leq 0$$
$$\lambda_3 + \mu_{n-1} \leq 0.$$

Since both λ_2, λ_3 are positive numbers, $\mu_n, \mu_{n-1} < 0$. In this case, the above equations can be written as:

$$\lambda_2^2 \leq \mu_n^2$$
$$\lambda_3^2 \leq \mu_{n-1}^2.$$

By Perron-Frobenius Theorem we have $|\mu_n| \leq |\mu_{n-1}| \leq \mu_1$. Equivalently, $\mu_n^2 \leq \mu_{n-1}^2 \leq \mu_1^2$. Therefore:

$$\begin{aligned}\mu_n^2 + \mu_{n-1}^2 &\leq \frac{2}{3}(\mu_n^2 + \mu_{n-1}^2 + \mu_1^2) \\ &\leq \frac{2}{3}\sum_{i=1}^{n} \mu_i^2 = \frac{2}{3}2|E(\bar{G})| \\ &= \frac{4}{3}(\binom{n}{2} - |E(G)|) \\ &< \frac{4}{3}(\frac{1}{2}n^2 - |E(G)|).\end{aligned}$$

So, we can deduce that :

$$\lambda_2^2 + \lambda_3^2 < \frac{4}{3}(\frac{n^2}{2} - |E(G)|)$$

or equivalently

$$\frac{3}{2}(\lambda_2^2 + \lambda_3^2) < n^2 - 2|E(G)|.$$

On the other hand, we have

$$\lambda_1^2 + \lambda_2^2 + \lambda_3^2 \leq 2|E(G)|.$$

By adding these two inequalities we have:

$$\lambda_1^2 + \frac{5}{2}\lambda_2^2 + \frac{5}{2}\lambda_3^2 < n^2.$$

Now, if we use Cauchy-Schwartz inequality, we can derive the following upper bound :

$$(\lambda_1 + \lambda_2 + \lambda_3)^2 \leq (\lambda_1^2 + \frac{5}{2}\lambda_2^2 + \frac{5}{2}\lambda_3^2)(1 + \frac{2}{5} + \frac{2}{5}) < \frac{9}{5}n^2.$$

Therefore,

$$\lambda_1 + \lambda_2 + \lambda_3 < \frac{3}{\sqrt{5}}n.$$

This shows that $\tau_3 \leq \frac{3}{\sqrt{5}}$. $\square$

In fact, the same argument can be done for any τ_k. The upper bound which can be obtained this way is $\tau_k \leq \frac{k}{\sqrt{2k-1}}$. But unfortunately, this bound is an improvement for the upper bound of 2.1.5, only for $k = 2, 3$.

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