ON THE SUM OF k LARGEST EIGENVALUES OF GRAPHS AND SYMMETRIC MATRICES

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Abstract

Let k be a positive integer and let G be a graph of order $n \geq k$. It is proved that the sum of k largest eigenvalues of G is at most $\frac{1}{2}(\sqrt{k}+1)n$. This bound is shown to be best possible in the sense that for every k there exist graphs whose sum is $\frac{1}{2}(\sqrt{k}+\frac{1}{2})n - o(k^{-2/5})n$. A generalization to arbitrary symmetric matrices is given.

1 Introduction

If G is a graph of order n, let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of its adjacency matrix $A = A(G)$, listed in the decreasing order. In this paper we consider the sum

$$\Lambda_k(G) = \lambda_1 + \lambda_2 + \cdots + \lambda_k$$

of k largest eigenvalues of the graph, where $1 \leq k \leq n$.

Study of the behavior of $\Lambda_k(G)$ for large values of k, in particular for $k = \lfloor \frac{n}{2} \rfloor$, is of interest in theoretical chemistry. Roughly speaking, eigenvalues of molecular graphs of (conjugated) hydrocarbons correspond to energy

levels of π-electrons, and the corresponding eigenvectors describe electron orbitals. Therefore, the sum of the largest eigenvalues, which correspond to orbitals with lowest energy levels, determine the total energy of the electrons. Since the quantity $\Lambda_{\lfloor \frac{n}{2} \rfloor}(G)$ is harder to handle analytically, Gutman introduced the related concept of the *energy* of a graph, $\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|$ to approximate $\Lambda_{\lfloor \frac{n}{2} \rfloor}(G)$. Observe that $\mathcal{E}(G) = 2\Lambda_{\lfloor \frac{n}{2} \rfloor}(G)$ if G is bipartite, since eigenvalues of a bipartite graph come in pairs, $\lambda_i = -\lambda_{n-i+1}$. Today, there is a vast literature in this area. We refer the reader to surveys [8, 9].

Another motivation to study the quantity $\Lambda_k(G)$ came from a result of Gernert [6], who proved that $\Lambda_2(G) \leq n$ if G is a regular graph of order n. He conjectured that this inequality holds for all graphs. Gernert's conjecture was disproved by Nikiforov [11], who gave examples of graphs with $\Lambda_2(G) \geq \frac{29+\sqrt{329}}{42}n - 25 > 1.122n - 25$ and proved that $\Lambda_2(G) \leq \frac{2}{\sqrt{3}}n < 1.155n$. A year later, Ebrahimi et al. [4] (independently) discovered new counterexamples to Gernert's conjecture and improved the lower bound of Nikiforov:

Theorem 1.1 ([4, 11]) *If G is a graph of order n, then*

$$\frac{1}{n}(\lambda_1 + \lambda_2) \leq \frac{2}{\sqrt{3}} < \frac{8.083}{7}.$$

For every $n \equiv 0 \bmod 7$, there exists a graph of order n with $\lambda_1 + \lambda_2 = \frac{8}{7}n - 2$.

We will study the sum of k largest eigenvalues in a more general setting by considering arbitrary symmetric matrices of order n. We denote this set by $\mathcal{S}_n = \{A \in \mathbb{R}^{n \times n} \mid A^T = A\}$. However, our main interest is in symmetric $n \times n$ matrices whose entries are between 0 and 1. We will denote this set by

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

For $1 \leq k \leq n$, we define

$$\tau_k(n) = \sup\{\tfrac{1}{n}\Lambda_k(A) \mid A \in \mathcal{M}_n\} \tag{1}$$

and

$$\tau_k = \limsup_{n \to \infty} \tau_k(n). \tag{2}$$

Theorem 1.1 shows that $\frac{8}{7} \leq \tau_2 < \frac{8.083}{7}$. It is also easy to see that $\tau_k \leq \tau_{k+1}$ for every $k \geq 1$.

Let us first make a rather straightforward observation that for the study of the quantity τ_k it suffices to consider 01-matrices, and in particular the adjacency matrices of graphs. This is stated formally in the next result. We denote by $\mathcal{G}_n \subseteq \mathcal{M}_n$ the set of all adjacency matrices of graphs of order n.

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Proposition 1.2 *For every integer $k \geq 1$, we have*

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

Proof. It is easy to see that it suffices to prove the following claim. For every integer n, every $\varepsilon > 0$, and every $A \in \mathcal{M}_n$, there exists an integer $N = N(A, \varepsilon)$ such that for every integer $r \geq 1$ there is a matrix $A^{(r)} \in \mathcal{G}_{rN}$ such that $\tau_k(A^{(r)}) \geq \tau_k(A) - \varepsilon$.

Let n, ε, A, and r be as above. Since $\tau_k(A)$ is a continuous function of the entries of A, there exists a rational matrix $B \in \mathcal{M}_n$ such that $\tau_k(B) \geq \tau_k(A) - \frac{\varepsilon}{2}$. Let q be the least common multiple of the denominators of all rational entries of B, and let $N = nq$. For $1 \leq i \leq n$ and $1 \leq j \leq n$, let $d_{ij} = rqB_{ij}$. Clearly, d_{ij} is an integer that is smaller or equal to rq. Let C_{ij} be a symmetric 01-matrix of order rq, in which each row and each column contains precisely d_{ij} 1's. (It is easy to see that such matrices exist.) Finally, let C be the matrix of order $rN = nrq$, which is composed of blocks C_{ij}, $1 \leq i \leq n$, $1 \leq j \leq n$.

It is easy to see that every eigenvalue $\lambda_i(B)$ of the matrix B gives rise to the eigenvalue $\nu_i = rq\lambda_i(B)$ of C. (The corresponding eigenvector is just a "lift" of an eigenvector of B.) Therefore,

$$\tau_k(C) \geq \frac{1}{nrq}\sum_{i=1}^{k}\nu_i = \frac{1}{n}\sum_{i=1}^{k}\lambda_i(B) = \tau_k(B) \geq \tau_k(A) - \frac{\varepsilon}{2}.$$

Clearly, C is a 01-matrix, but it may happen that $C \notin \mathcal{G}_{rN}$ since its diagonal entries may be nonzero. However, we set $A^{(r)} \in \mathcal{G}_{rN}$ to be the matrix obtained from C by replacing all diagonal elements with zeros. Then it is easy to see that $\lambda_i(A^{(r)}) \geq \lambda_i(C) - 1$. Thus, if we take N to be larger than $2n\varepsilon^{-1}$, we conclude that

$$\tau_k(A^{(r)}) \geq \tau_k(C) - \frac{k}{rN} \geq \tau_k(C) - \frac{\varepsilon}{2} \geq \tau_k(A) - \varepsilon.$$

$\square$

Trivially, $\tau_k \leq k$. It is also easy to prove that $\tau_k \leq \sqrt{k}$, simply by using the Cauchy-Schwartz inequality. The main result of this note is an improved upper bound for τ_k:

Theorem 1.3 *For every integer $k \geq 2$, we have $\tau_k \leq \frac{1}{2}(1 + \sqrt{k})$.*

The proof of the theorem is given in Section 2.

For $k = 2$, the bound of Theorem 1.3 is weaker than Nikiforov's bound in Theorem 1.1. It is also unlikely that it is best possible for other values of k. However, examples provided in Section 3 show that the bound of Theorem 1.3 is essentially best possible if k is large enough.

Theorem 1.4 *Let q be an odd prime power and let $k = q^2 - q + 1$. Then*

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

The proofs of this result and of the following corollary, which describes almost exact asymptotic behavior of τ_k, are given in Section 3.

Corollary 1.5 *For every $k \geq 2$ we have*

$$\tfrac{1}{2}\left(\sqrt{k} + \tfrac{1}{2}\right) - o(k^{-2/5}) \leq \tau_k \leq \tfrac{1}{2}(1 + \sqrt{k}).$$

By shifting and scaling, Theorem 1.3 implies a result which holds for the sum of k largest (or smallest) eigenvalues of an arbitrary symmetric matrix.

Theorem 1.6 *If a, b are real numbers, where $a < b$, and n is an integer, let $\mathcal{S}_n^{a,b}$ be the set of all matrices $A \in \mathcal{S}_n$ whose entries are between a and b. Then for every integer k, $2 \leq k \leq n$, and every $A \in \mathcal{S}_n^{a,b}$ we have*

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

Proof. Let Q be the all-1-matrix, and consider the matrix $B = A - aQ$. Then $\frac{1}{b-a} B \in \mathcal{M}_n$. By Theorem 1.3,

$$\sum_{i=1}^{k} \lambda_i(B) \leq \frac{n}{2}(1 + \sqrt{k})(b - a). \tag{3}$$

It is known that largest eigenvalues of the sum of two matrices are majorized by the sum of the eigenvalues of the two matrices (cf., e.g., [10, Theorem 4.3.27]). In our case this gives:

$$\sum_{i=1}^{k} \lambda_i(A) \leq \sum_{i=1}^{k} \lambda_i(B) + \sum_{i=1}^{k} \lambda_i(aQ). \tag{4}$$

Since $\sum_{i=1}^{k} \lambda_i(aQ)$ is at most 0 if $a \leq 0$, and is equal to an if $a \geq 0$, the inequality of the theorem follows from (3) and (4). $\square$

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2 Proofs

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

$$\sigma_2(A) = \left(\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} |A_{ij}|^2 \right)^{1/2}.$$

We shall need an estimate on the eigenvalues of A in terms of $\sigma_2(A)$.

Lemma 2.1 *If $A \in \mathcal{S}_n$ has eigenvalues $\lambda_1, \ldots, \lambda_n$, then*

$$\lambda_1^2 + \lambda_2^2 + \cdots + \lambda_n^2 = 2\big(\sigma_2(A)\big)^2.$$

Proof. Since A is symmetric, we have $(A^2)_{ii} = \sum_{j=1}^{n} A_{ij}^2$. Therefore, $2\sigma_2(A)^2 = \mathrm{tr}(A^2) = \sum_{i=1}^{n} \lambda_i^2$. $\qquad\square$

Let $q = (q_1, \ldots, q_n)^T$ and $Q = qq^T$. Then Q is a symmetric matrix of rank 1 with its only nontrivial eigenvalue $\kappa = \mathrm{tr}(Q) = \|q\|^2$. Clearly, the corresponding eigenvector is q.

Given a matrix $A \in \mathcal{S}_n$, we define its *q-complement* as the matrix A', defined by $A' = Q - A$, where $Q = qq^T$ is as above. 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'.

Lemma 2.2 (a) $\lambda_1 + \lambda_1' \geq \|q\|^2$.
    (b) $\lambda_i + \lambda_{n-i+2}' \leq 0$ *for $i = 2, 3, \ldots, n$.*

Proof. Part (b) is a version of Weyl inequalities; we give a self-contained proof for completeness. Let us recall the Courant-Fischer min-max characterization of the ith eigenvalue of a symmetric matrix:

$$\lambda_i = \min_U \max_{x \in U, \|x\|=1} \langle Ax, x \rangle \qquad (5)$$

where the minimum is taken over all $(n - i + 1)$-dimensional subspaces U of $\mathbb{R}^n$. Now, let $y_1, \ldots, y_{i-2}$ be the eigenvectors of A' corresponding to the smallest $i - 2$ eigenvalues. If U' is an $(n - i + 1)$-dimensional subspace of $\mathbb{R}^n$ which is orthogonal to all vectors $y_1, \ldots, y_{i-2}$, then $\langle A'x, x \rangle \geq \lambda_{n-i+2}'$ for every $x \in U'$ with $\|x\| = 1$. If we also ask that U' is orthogonal to q, then $\langle Qx, x \rangle = 0$ for every $x \in U'$. By restricting the minimum in (5) only to spaces U' that are orthogonal to $y_1, \ldots, y_{i-2}$ and to q (if q is not a

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linear combination of y's, then U' is uniquely determined), then we get the inequality

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

This proves (b).

To prove (a), observe that $\mathrm{tr}(A) + \mathrm{tr}(A') = \mathrm{tr}(Q) = \|q\|^2$. Therefore

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

By using (b), inequality (a) follows. $\qquad\square$

We are now ready for the proof of Theorem 1.3. By Proposition 1.2, it suffices to prove that the adjacency matrix of any graph of order $n \geq k$ satisfies $\tau_k(A) \leq \frac{1}{2}(1 + \sqrt{k})$. By using the above notation, let us define $\alpha = (\frac{1}{n}\sigma_2(A))^2$ and $\alpha' = (\frac{1}{n}\sigma_2(A'))^2$, where A' is the q-complement of A. At this point we will take $q = (1, \ldots, 1)^T$, so Q is the all-1-matrix, and $\|q\|^2 = n$. Then

$$
\begin{aligned}
\alpha + \alpha' \quad &= \quad \frac{1}{2n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} (A_{ij}^2 + (1 - A_{ij})^2) \\
&= \quad \frac{1}{2n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} (1 + 2A_{ij}^2 - 2A_{ij}) \\
&= \quad \frac{1}{2}. \tag{6}
\end{aligned}
$$

Let us define $\nu_i = \max\{0, \lambda_i\}$. Lemma 2.2 implies that $\nu_i^2 \leq \lambda'^2_{n-i+2}$ for $i = 2, \ldots, n$. Part (a) of the same lemma shows that $\lambda_1 + \lambda'_1 \geq n$. By setting $t = \frac{1}{n}\lambda_1$, we derive therefrom that

$$
\lambda_1^2 + \lambda_1'^2 \geq t^2 n^2 + (1 - t)^2 n^2 = (1 - 2t(1 - t))n^2. \tag{7}
$$

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The above inequalities will be used in the following estimates:

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

This shows that $\sum_{i=2}^{k} \nu_i^2 \leq t(1-t)n^2$. An application of the Cauchy-Schwartz inequality now yields:

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

Therefore,

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

Finally, we conclude that

$$
\tau_k(A) \leq t + \sqrt{(k-1)t(1-t)}. \tag{8}
$$

The parameter t in (8) is between 0 and 1, and a routine calculation shows that the right hand side has maximum value at $t = \frac{1}{2}(1 + k^{-1/2})$. The value at this point is equal to $\frac{1}{2}(1 + k^{1/2})$, so we conclude that

$$
\tau_k(A) \leq \frac{1}{2}(1 + \sqrt{k}). \tag{9}
$$

This completes the proof of Theorem 1.3.

3 Examples

The proof of Theorem 1.3 shows that graphs whose sum of the largest k eigenvalues would be close to the derived upper bound, will have eigenvalues $\lambda_2, \ldots, \lambda_k$ close to $\frac{1}{2} n k^{-1/2}$, and their complements will have smallest eigenvalues close to $-\frac{1}{2} n k^{-1/2}$. There are some well studied familes of graphs whose eigenvalues exhibit such "extreme" behavior. We shall examine them in more detail in order to provide lower bounds on τ_k. In particular, we shall prove Theorem 1.4 and Corollary 1.5. We are assuming basic familiarity with the notion of strongly regular graphs and refer to [3] or [7] for details.

Taylor [14] described a construction of strongly regular graphs, which are known today as *Taylor graphs*, cf. [3]. They are related to the notion of two-graphs. We shall need a family of Taylor graphs (originally described in [13]) that can be obtained as follows.

Let q be an odd prime power, and let H be a non-degenerate Hermitian form in $\mathrm{PG}(2, q^2)$ with the corresponding Hermitian curve U. Note that $|U| = q^3 + 1$. Let Δ be the set of triples $\{x, y, z\}$ from U such that $H(x, y)H(y, z)H(z, x)$ is a square in the field $\mathrm{GF}(q^2)$ if $q \equiv 3 \pmod 4$, and is a non-square in $\mathrm{GF}(q^2)$ if $q \equiv 1 \pmod 4$. Let $\mathcal{H}(q)$ be the set of all graphs G with vertex set U such that the triple $\{x, y, z\}$ of vertices is in Δ if and only if x, y, z induce a subgraph with an odd number (i.e., eithe 1 or 3) of edges. Taylor proved that $\mathcal{H}(q)$ is non-empty and that for every $u \in U$, there is a unique graph $G_u \in \mathcal{H}(q)$, in which the vertex u has degree 0. Its vertex-deleted subgraph $H'_q = G_u - u$ is one of the Taylor graphs. It is a strongly regular graph of order $n = q^3$ and with parameters $\left(q^3, \frac{1}{2}(q-1)(q^2+1), \frac{1}{4}(q-1)^3 - 1, \frac{1}{4}(q-1)(q^2+1)\right)$. Finally, the complement $\overline{H'_q}$ of H'_q is also a strongly regular graph. Its parameters can be easily computed:

$$\left(q^3, \tfrac{1}{2}(q+1)(q^2-1), \tfrac{1}{4}(q+3)(q^2-3) + 1, \tfrac{1}{4}(q+1)(q^2-1)\right).$$

The parameters of a strongly regular graph determine its eigenvalues and their multiplicities (cf., e.g., [7, Section 10.2]). The eigenvalues are $\lambda_1 = \frac{1}{2}(q+1)(q^2-1)$ (simple eigenvalue), $\lambda_2 = \frac{1}{2}(q^2-1)$ (with multiplicity $q(q-1)$), and $\lambda_n = -\frac{1}{2}(q+1)$ (with multiplicity $(q-1)(q^2+1)$). So, if we take $k = q^2 - q + 1$, we get

$$
\begin{aligned}
\tau_k(\overline{H'_q}) &= \frac{1}{2q^3}(q+1)(q^2-1) + \frac{1}{2q^3}(q^2-1) \cdot q(q-1) \\
&= \frac{q^4 - 1}{2q^3}.
\end{aligned}
$$

A routine calculation now gives the following lower bound on $\tau_k(\overline{H_q'})$

$$\tau_k(\overline{H_q'}) \geq (\sqrt{k} + 1)\left(\tfrac{1}{2} - \tfrac{1}{4}k^{-1/2} + \tfrac{1}{16}k^{-1} - \tfrac{1}{16}k^{-3/2} + O(k^{-2})\right) \qquad (10)$$

if $k = q^2 - q + 1$ and q is an odd prime power. This completes the proof of Theorem 1.4.

Since there is a prime between every integer x and $x + o(x^{3/5})$ (see, e.g., [2]) and since τ_k is non-decreasing in terms of k, we conclude from (10) that

$$\tau_k \geq (\sqrt{k} + 1)\left(\tfrac{1}{2} - \tfrac{1}{4}k^{-1/2} - o(k^{-9/10})\right)$$

for every k. This yields Corollary 1.5.

At the end we provide some further families of graphs and estimates for the values of $\tau_k(G)$ which may be of certain interest.

Let n be a prime that is congruent to 1 modulo 4. The Paley graph $\mathbf{P}_n$ of order n has vertex set $V = \{0, \ldots, n-1\}$, and two vertices $i, j \in V$ are adjacent if and only if $i - j$ is a non-zero square modulo n, i.e., $i \neq j$ and there exists an integer x such that $i - j \equiv x^2 \pmod{n}$. It is well known that $\mathbf{P}_n$ is a strongly regular graph with eigenvalues $\lambda_1 = \frac{n-1}{2}$ and $\lambda_i = \frac{1}{2}(\sqrt{n}-1)$ for $i = 2, \ldots, k$, where $k = \frac{n-1}{2}$; see, e.g., [7] for details. Therefore,

$$\tau_k(\mathbf{P}_n) = \frac{n-1}{2n} + \frac{k-1}{2n}(\sqrt{n} - 1) = \frac{1}{4}(\sqrt{n} + 1) - o(1).$$

This implies that

$$\tau_k \geq \frac{1}{4}(\sqrt{2k+1} + 1). \qquad (11)$$

Somewhat similar eigenvalue behavior can be found in the Latin square graphs (see [7, Section 10.4]). If $OA(N, d)$ is an orthogonal array, it defines a strongly regular graph with parameters $(N^2, d(N-1), N-2+(d-1)(d-2), d(d-1))$ (see, e.g., [7] for definitions). The "extremal" behavior with respect to τ_k in this family of graphs is achieved for $d \approx \frac{1}{3}N$, where it gives the bound

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

for $k = d(N - 1)$. Orthogonal arrays with d as large as $\frac{1}{3}N$ exist if N is a prime power, and the added factor $(1 + o(1))$ compensates for the missing values of k.

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Random graphs exhibit similar eigenvalue behavior as Paley graphs, but provide slightly weaker estimates for τ_k. Nevertheless, these are interesting examples, and we shall provide some more details.

The largest eigenvalue of random graphs $\mathcal{G}(n, 1/2)$ is almost surely close to $\frac{n}{2}$, and all other eigenvalues almost surely have absolute value $O(\sqrt{n})$. This was proved by Füredi and Komlós [5]. Wigner's paper [15] gives the density of the eigenvalue distibution of random graphs (see also [1]). Wigner's semicircle law shows that the number of eigenvalues that are greater than $t\sqrt{2n}$ is approximately equal to

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

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 $t_0 = 0.293435$ (for which experiments show to give almost best possible bound), we obtain the following lower bound for $k = k_n(t_0)$:

$$\tau_k \geq \frac{s_n(t_0)}{n}(1 + o(1)) > 0.32985\sqrt{k}\,(1 + o(1)).$$

There is a strongly regular graph with parameters (276,135,78,54), known also as the Conway-Goethals-Seidel graph. This graph is described in [7, p. 263]. For $k = 24$ it gives

$$\tau_k > 0.4643397(\sqrt{k} + 1).$$

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

Table 1: Some strongly regular graphs give extremal behavior for τ_k.

Among small strongly regular graphs, there are even better candidates. Some feasible parameters (taken from the list calculated by Gordon Royle

[12]) give constants quite close to $\frac{1}{2}$. Some of them are collected in Table 1. The table shows the parameters of the selected strongly regular graph, the corresponding value of k, and the value of $\tau_k(G)/(\sqrt{k}+1)$ for this graph.

References

[1] L. Arnold, On the asymptotic distribution of the eigenvalues of random matrices, J. Math. Anal. Appl. 20 (1967) 262–268.

[2] R. C. Baker, G. Harman, and J. Pintz, The exceptional set for Goldbach's problem in short intervals, in "Sieve Methods, Exponential Sums, and Their Applications in Number Theory (Cardiff, 1995)," Cambridge Univ. Press, Cambridge, 1997, pp. 1–54.

[3] A. E. Brouwer, A. M. Cohen, and A. Neumaier, Distance-Regular Graphs, Springer-Verlag, 1989.

[4] J. Ebrahimi B., B. Mohar, and A. Sheikh Ahmady, On the sum of two largest eigenvalues of a graph, submitted.

[5] Z. Füredi and J. Komlós, The eigenvalues of random symmetric matrices, Combinatorica 1 (1981) 233–241.

[6] D. Gernert, private communication, see also `http://www.sgt.pep.ufrj.br/home_arquivos/prob_abertos.html`

[7] C. Godsil, G. Royle, Algebraic Graph Theory, Springer, 2001.

[8] I. Gutman, The energy of a graph: Old and new results, in "Algebraic Combinatorics and Applications," A. Betten, A. Kohner, R. Laue, and A. Wassermann, eds., Springer, Berlin, 2001, pp. 196–211.

[9] I. Gutman, O. E. Polansky, Mathematical Concepts in Organic Chemistry, Springer, Berlin, 1986, pp. 135-154.

[10] R. A. Horn, C. R. Johnson, Matrix Analysis, Cambridge Univ. Press, Cambridge, 1985.

[11] V. Nikiforov, Linear combinations of graph eigenvalues, Electr. J. Linear Algebra 15 (2006) 329–336.

[12] G. Royle, Parameters for strongly regular graphs of order less than 1000, `http://people.csse.uwa.edu.au/gordon/remote/srgs/index.html`

[13] D. E. Taylor, Some topics in the theory of finite groups, Ph.D. Thesis, University of Oxford, 1971.

[14] D. E. Taylor, Regular 2-graphs, Proc. London Math. Soc. 35 (1977) 257–274.

[15] E. P. Wigner, On the distribution of the roots of certain symmetric matrices, Ann. Math. 67 (1958) 325–327.