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On the sum of two largest eigenvalues of a symmetric matrix

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Abstract

D. Gernert conjectured that the sum of two largest eigenvalues of the adjacency matrix of any 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 one of the authors [4], who also provided a nontrivial upper bound for the sum of two largest eigenvalues. In this paper we improve the lower and upper bounds to near-optimal ones, and extend results from graphs to general non-negative matrices.

1 Introduction

It is of interest to know which symmetric matrices have "extremal" eigenvalue behavior. In this paper we consider the sum of two largest eigenvalues of a symmetric matrix of order n, and we ask how large can this sum be, and what can we say about (nearly) "extremal" matrices. Gernert [1] proposed the following:

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Conjecture 1.1 (Gernert [1]) *If G is a simple graph of order n and λ_1 and λ_2 are the two largest eigenvalues of G, then $\lambda_1 + \lambda_2 \leq n$.*

Gernert proved that the inequality $\lambda_1 + \lambda_2 \leq n$ holds for all regular graphs and has verified it for several other classes of graphs, such as planar, toroidal, complete multipartite and triangle-free graphs.

We will study the sum of largest eigenvalues in a more general setting by considering the set of non-negative symmetric $n \times n$ matrices whose entries are between 0 and 1. We will denote this set by

$$\mathcal{M}_n = \{A \in \mathbb{R}^{n \times n} \mid A^T = A,\, 0 \leq a_{ij} \leq 1 \text{ for } 1 \leq i, j \leq n\}.$$

We let $\lambda_i = \lambda_i(A)$ be the ith largest eigenvalue (counting multiplicities) of the matrix $A \in \mathcal{M}_n$ and define

$$\tau_2(A) = \frac{1}{n}(\lambda_1(A) + \lambda_2(A)).$$

We will be interested in extremal values of the quantity

$$\tau_2(n) = \sup\{\tau_2(A) \mid A \in \mathcal{M}_n\}$$

and its asymptotic behavior

$$\tau_2 = \limsup_{n \to \infty} \tau_2(n).$$

First of all, we shall extend Gernert's result mentioned above by proving that for every matrix $A \in \mathcal{M}_n$ with constant row sums we have $\tau_2(A) \leq 1$. In particular, for any regular graph G of order n we have $\lambda_1 + \lambda_2 \leq n - 2$, with equality if and only if the complement of the graph G has a connected component that is bipartite; cf. Corollary 3.2.

Next, a construction of simple graphs of order n (where $n \equiv 0 \pmod 7$) with $\lambda_1 + \lambda_2 = \frac{8}{7}n - 2$ is given. Apparently, this is a counterexample to Conjecture 1.1. Such counterexamples were found earlier by one of the authors [4], but they were not as tight as the current one for which we believe that it might be the extreme case. The same author also found a non-trivial upper bound in [4]; he proved that for every n, $\tau_2(n) \leq 2/\sqrt{3}$.

In this paper we provide an improved upper bound that is very close to our lower bound. We also show that the same bounds hold for arbitrary matrices in $\mathcal{M}_n$.

Theorem 1.2 *If $A \in \mathcal{M}_n$, then*

$$\tau_2(A) \le \tfrac{1}{2} + \sqrt{\tfrac{5}{12}} < \frac{8.0185}{7}.$$

For every $n \equiv 0 \pmod 7$, there exists a graph G_n of order n with $\lambda_1(G_n) + \lambda_2(G_n) = \frac{8}{7}n - 2$. In particular, $\tau_2 \ge \frac{8}{7}$.

The proof of the upper bound is provided in Section 4 and the construction of graphs claimed for in Theorem 1.2 is given in Section 2.

Recently one of the authors [3] considered the problem of how large can be the sum of k largest eigenvalues of a graph (or a symmetric matrix). As shown in [3], the bounds of Theorem 1.2 can be used, by shifting and scaling the matrices, to get a result which holds for the sum of the largest (or the smallest) two eigenvalues of an arbitrary symmetric matrix.

Corollary 1.3 *Let a, b are real numbers, where $a < b$, and let A be a symmetric matrix, all of whose entries are between a and b. Then*

$$\tau_2(A) \le \tfrac{1}{2}\Big(1 + \sqrt{\tfrac{5}{3}}\Big)(b - a) + \max\{0, a\}.$$

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 extremal examples for the value of $\tau_2(7n)$.

Let $n \ge 1$ 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 the 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 2.1 *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 X, Y, Z be as above. It is convenient to consider the matrix $B = A(G_n) + I$, whose rank is three since its rows corresponding to the vertices in X (resp. in Y or Z) are the same. Thus it suffices to see that B has eigenvalues $6n$, $2n$, and $-n$.

Suppose that $f : V \to \mathbb{R}$ is a function whose values are constant on each part X, Y, Z. Let $f(v) = x$ for $v \in X$, $f(v) = y$ for $v \in Y$, and $f(v) = z$ for $v \in Z$. Then f is an eigenfunction corresponding to an eigenvalue μ of B if and only if the following equations hold:

$$\begin{aligned} \mu x &= 2nx + 3ny \\ \mu y &= 2nx + 3ny + 2nz \\ \mu z &= 3ny + 2nz. \end{aligned}$$

This homogeneous system of linear equations has three solutions for μ such that $\{x, y, z\} \neq \{0\}$. They are $\mu_1 = 6n$, $\mu_2 = 2n$, and $\mu_3 = -n$. This gives three solutions $6n - 1$, $2n - 1$, and $-n - 1$ for eigenvalues of G_n, as claimed.

□

3 Matrices with constant row sums

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

$$\sum_{j=1}^{n} a_{ij} = r$$

holds for some constant r ($0 \leq r \leq n$) and for every $i = 1, \ldots, n$. For example, the adjacency matrix of an r-regular graph of order n is such a matrix.

For $A \in \mathcal{M}_n$, define the matrix $A' = J - A$, where J is the all-1-matrix of order n. Let $j = (1, 1, \ldots, 1)^T \in \mathbb{R}^n$. One can easily see that j is an eigenvector of both matrices, A and A', corresponding to the eigenvalues r and $n - r$, respectively. Moreover, these are the largest eigenvalues of these two matrices.

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

$$Au + A'u = Ju = j\,j^T u = 0.$$

This implies that $Au = -A'u$. The same argument works if we interchange the role of A and A'. Hence, the second largest eigenvalue of A is not bigger than the negative of the smallest eigenvalue of A'. On the other hand, the Perron-Frobenius Theorem implies that the smallest eigenvalue of A' has absolute value not larger than the largest eigenvalue $n-r$ of A'. Hence, the second largest eigenvalue of A is at most $n-r$ and therefore $\tau_2(A) \leq \frac{1}{n}(r+(n-r)) = 1$. This proves the following proposition:

Proposition 3.1 *If $A \in \mathcal{M}_n$ has constant row sums, then $\tau_2(A) \leq 1$.*

Corollary 3.2 *If G is a regular graph of order n, then the sum of two largest eigenvalues λ_1, λ_2 of G is at most $n-2$. Moreover, $\lambda_1+\lambda_2 = n-2$ if and only if the complement of G has a connected component which is bipartite.*

Proof. Apply the previous proposition to the matrix $A+I$ where A is the adjacency matrix of G and I is the identity matrix of size n.

It remains to verify the claim when equality holds. Let r be the vertex degree in G. Let $q = n-r-1$. The complement H of G is q-regular. If it has a bipartite component, then H has eigenvalues $\lambda'_1 = q$ and $\lambda'_n = -q$. An eigenvector of λ'_n is easily seen to be an eigenvector of G for the eigenvalue $\lambda = q-1$. Therefore, $\tau_2(G) \geq r+\lambda = n-2$, and so we have equality. Conversely, the proof of Proposition 3.1 shows that when equality occurs, the smallest eigenvalue of H is $-(n-r)$, and by the Perron-Frobenius Theorem we conclude that a connected component of H is bipartite. $\square$

4 Upper bound

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

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

Since $(A^2)_{ii} = \sum_{j=1}^{n} a_{ij}^2$, we have

$$2\sigma_2(A)^2 = \mathrm{tr}(A^2) = \sum_{i=1}^{n} \lambda_i^2, \tag{1}$$

where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of A in decreasing order.

Let $A' = J - A$, where J is the all-1 matrix of order n, and let $\lambda'_1 \geq \lambda'_2 \geq \cdots \geq \lambda'_n$ be the eigenvalues of A'.

The following inequalities are special cases of Weyl inequalities (cf., e.g., [2, Theorem 4.3.1]) applied to matrices A, A', and $J = A + A'$.

Lemma 4.1 (a) $\lambda_2 + \lambda'_n \le 0$. (b) $\lambda_i + \lambda'_{n-i+1} \ge 0$, *for* $i = 1, \ldots, n$.

We shall need two additional ingredients. The first one shows that matrices with extreme values of τ_2 are adjacency matrices of graphs (with loops), whose complement is bipartite.

Lemma 4.2 *Let* $A \in \mathcal{M}_n$. *Then there exists a graph* G *of order* n *(with the loop at each vertex) whose complement is a bipartite graph, and such that* $\tau_2(G) \ge \tau_2(A)$.

Proof. Let $V = \{1, \ldots, n\}$ and let x and y be orthonormal eigenvectors for $\lambda_1(A)$ and $\lambda_2(A)$, respectively, whose entries are indexed by V. Let $B = \{v \in V \mid y_v = 0\}$, $C = \{v \in V \mid y_v > 0\}$, and $D = \{v \in V \mid y_v < 0\}$. Let G be the graph with vertex set V, whose edges are all pairs $\{u, v\}$ (including loops) for which one of the following holds:
(1) $u, v \in B \cup C$, or
(2) $u, v \in B \cup D$, or
(3) $u \in C$, $v \in D$ and $x_u x_v + y_u y_v \ge 0$.
Clearly, the complement of G has only edges joining vertices of C and D, and is thus bipartite. By the Perron-Frobenius Theorem, we have $x_v \ge 0$ for every $v \in V$. Therefore, the definition of the sets B, C, and D implies that

$$x^T A(G) x + y^T A(G) y = 2 \cdot \sum_{uv \in E(G)} (x_u x_v + y_u y_v) \ge x^T A x + y^T A y.$$

Using this inequality and the Ky Fan inequality (see [2, Corollary 4.3.18]) for the sum of two largest eigenvalues of $A(G)$, we get:

$$\begin{aligned} \lambda_1(G) + \lambda_2(G) &= \max_{\|z\|=1, \|w\|=1, z \perp w} (z^T A(G) z + w^T A(G) w) \\ &\ge x^T A(G) x + y^T A(G) y \\ &\ge x^T A x + y^T A y \\ &= \lambda_1(A) + \lambda_2(A), \end{aligned}$$

which we were to prove. $\square$

Lemma 4.3 *If a graph* G *of order* $n \ge 4$ *has bipartite complement, then*

$$\lambda_1(G) + \lambda_2(G) + \lambda_{n-1}(G) + \lambda_n(G) \le n.$$

Proof. Using Lemma 4.1(b), we can estimate:

$$\begin{aligned} n &\geq \operatorname{tr}(A(G)) = \lambda_1 + \lambda_2 + \lambda_{n-1} + \lambda_n + \sum_{i=3}^{n-2} \lambda_i \\ &\geq \lambda_1 + \lambda_2 + \lambda_{n-1} + \lambda_n + \sum_{i=3}^{n-2} \lambda'_{n-i+1} \\ &= \lambda_1 + \lambda_2 + \lambda_{n-1} + \lambda_n. \end{aligned}$$

The last equality is a consequence of the fact that $\lambda'_i = \lambda'_{n-i+1}$ for every i, since the complement of G is bipartite. □

We are now ready for the proof of Theorem 1.2. By Lemma 4.2, we may assume that A is the adjacency matrix of a graph G, with a loop at each vertex, whose complement is bipartite. We will use the notation introduced above.

We may assume that $\lambda_2 \geq 0$, since otherwise $\tau_2(A) \leq 1$. Equation (1) applied to matrices A and A' shows that

$$\begin{aligned} \sum_{i=1}^{n} \lambda_i^2 + \sum_{i=1}^{n} \lambda_i'^2 &= 2\sigma_2(A)^2 + 2\sigma_2(A')^2 \\ &= \sum_{i=1}^{n}\sum_{j=1}^{n} \left(a_{ij}^2 + (1-a_{ij})^2\right) = n^2. \end{aligned} \tag{2}$$

Since $\lambda_2 \geq 0$, Lemma 4.1(a) and bipartiteness of the complement imply that $\lambda_2^2 \leq \lambda_n'^2 = \lambda_1'^2$. Let us first assume that $\lambda_{n-1} \leq 0$. Then, similarly as above, Lemma 4.1(b) applied with $i = n-1$ shows that $\lambda_{n-1}^2 \leq \lambda_2'^2 = \lambda_{n-1}'^2$. Combining these inequalities and (2), we get:

$$\begin{aligned} \lambda_1^2 + 3\lambda_2^2 + 3\lambda_{n-1}^2 + \lambda_n^2 &\leq \lambda_1^2 + \lambda_2^2 + \lambda_{n-1}^2 + \lambda_n^2 + \lambda_1'^2 + \lambda_n'^2 + \lambda_2'^2 + \lambda_{n-1}'^2 \\ &\leq n^2. \end{aligned} \tag{3}$$

For $i = 1, \ldots, n$, let $t_i := \frac{1}{n}\lambda_i$. Lemma 4.3 gives

$$t_1 + t_2 + t_{n-1} + t_n \leq 1. \tag{4}$$

From (3) we see that

$$t_1^2 + 3t_2^2 + 3t_{n-1}^2 + t_n^2 \leq 1, \tag{5}$$

while our goal is to maximize $\tau := t_1+t_2$. By the Cauchy-Schwartz inequality we have

$$\tau^2 = (t_1+t_2)^2 \le (1+\tfrac{1}{3})(t_1^2+3t_2^2) = \tfrac{4}{3}(t_1^2+3t_2^2) \tag{6}$$

and similarly (by assuming $\tau \ge 1$ and using (4) first):

$$(\tau-1)^2 \le (t_{n-1}+t_n)^2 \le \tfrac{4}{3}(3t_{n-1}^2+t_n^2). \tag{7}$$

Using (5)–(7), we conclude that $\tau^2+(\tau-1)^2 \le \frac{4}{3}$. Solving this quadratic inequality, we obtain $\tau \le 1/2+\sqrt{5/12}$. This completes the proof of Theorem 1.2 when $\lambda_{n-1} \le 0$.

Suppose now that $\lambda_{n-1} \ge 0$ and that $\tau_2(A) \ge \frac{8}{7}$. Then Lemma 4.3 implies that $|\lambda_n| \ge \frac{1}{7}n$. Thus,

$$\lambda_1^2+3\lambda_2^2 \le \lambda_1^2+\lambda_2^2+\lambda_1'^2+\lambda_n'^2 \le n^2-\lambda_n^2 \le \tfrac{48}{49}n^2.$$

Consequently,

$$\tau^2 = (t_1+t_2)^2 \le \tfrac{4}{3}(t_1^2+3t_2^2) \le \tfrac{4}{3}\cdot\tfrac{48}{49} = (\tfrac{8}{7})^2.$$

The proof is now complete.

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