Czechoslovak Mathematical Journal

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Czechoslovak Mathematical Journal, Vol. 48 (1998), No. 1, 1–20

Persistent URL: http://dml.cz/dmlcz/127394

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BOUNDS ON THE SUBDOMINANT EIGENVALUE INVOLVING GROUP INVERSES WITH APPLICATIONS TO GRAPHS

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(Received October 10, 1994)

Abstract. Let A be an $n \times n$ symmetric, irreducible, and nonnegative matrix whose eigenvalues are $\lambda_1 > \lambda_2 \geqslant \ldots \geqslant \lambda_n$. In this paper we derive several lower and upper bounds, in particular on λ_2 and λ_n, but also, indirectly, on $\mu = \max\limits_{2 \leqslant i \leqslant n} |\lambda_i|$. The bounds are in terms of the diagonal entries of the group generalized inverse, $Q^{\#}$, of the singular and irreducible M-matrix $Q = \lambda_1 I - A$. Our starting point is a spectral resolution for $Q^{\#}$. We consider the case of equality in some of these inequalities and we apply our results to the algebraic connectivity of undirected graphs, where now Q becomes L, the Laplacian of the graph. In case the graph is a tree we find a graph-theoretic interpretation for the entries of $L^{\#}$ and we also sharpen an upper bound on the algebraic connectivity of a tree, which is due to Fiedler and which involves only the diagonal entries of L, by exploiting the diagonal entries of $L^{\#}$.

1. Introduction

Let A be an $n \times n$ nonnegative irreducible matrix whose eigenvalues are $\lambda_1, \ldots, \lambda_n$. Assume that the Perron root of A is λ_1, so that λ_1 is also its spectral radius. Let

$$\mu := \max_{i \neq 1} |\lambda_i|.$$

The importance of λ_1 in all sorts of applications, e.g., the convergence of iterative methods for solving nonsingular systems of equations in the presence of nonnegative

[1] Research supported in part by a University of Regina Grad Studies Special Project Grant and NSERC Grant No. OG0138251.
[2] Research supported by NSF Grant No. DMS-9306357.
[3] Research partially supported by NSA Grant No. MDA904-94-H-2051.

iteration matrices, is well known. But, for example, in iterative methods for solving singular systems, in the presence of a nonnegative iteration matrix whose powers converge, we have that $\lambda_1 = 1$ and it is μ which governs the asymptotic rate of convergence of the scheme, see, for example, Berman and Plemmons [2] and Neumann and Plemmons [12] and references therein. In the special case when A is a transition matrix for a regular Markov chain, μ serves as the *coefficient of ergodicity.* In this context μ measures the asymptotic rate at which the stationary distribution vector can be approached starting from an arbitrary initial distribution vector, see Seneta [14].

Subdominant eigenvalues of nonnegative matrices also arise in a graph-theoretic context. Specifically, suppose that $A = A(\mathcal{G})$ is an adjacency matrix of a loopless undirected graph $\mathcal{G}$. Let $D = D(\mathcal{G})$ be the diagonal matrix whose diagonal entries are the corresponding vertex degrees, where by the *degree of a vertex* is meant the number of edges incident to the vertex. The matrix $L = L(\mathcal{G}) := D - A$ is known as the *Laplacian of* $\mathcal{G}$. Let

$$d = \max_{1 \leqslant i \leqslant n} d_i.$$

Then L can be written as

$$L = dI - [\mathrm{diag}(d - d_1, \ldots, d - d_n) + A] =: dI - M.$$

Letting the eigenvalues of M be $d = \lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant \lambda_n$, we see that the eigenvalues of L are $0 \leqslant d - \lambda_2 \leqslant \ldots \leqslant d - \lambda_n$. Fiedler [5] has shown that $\mathcal{G}$ is a connected graph if and only if the second smallest eigenvalue of L (i.e. $d - \lambda_2$) is positive and he has used that quantity, which is called the *algebraic connectivity of* $\mathcal{G}$, as a measure of the connectivity of $\mathcal{G}$. We see then that once again the subdominant eigenvalue λ_2 comes into play. In various papers, see for example Merris [10] or Powers [13], upper and lower bounds for the degree of connectivity are developed. (We, in fact, refer the reader to the three papers [5], [10], and [13] for more background material on graph definitions and properties used in this paper.)

Recently Meyer [8] has obtained upper bounds on the *reciprocals* of certain extremal subdominant eigenvalues associated with ergodic Markov chains in terms of the so called group inverse associated with the chain. Let A be an irreducible stochastic matrix whose eigenvalues are $\lambda_1 = 1, \lambda_2, \ldots, \lambda_n$. Put $Q = I - A$ and let $Q^{\#}$ be its group generalized inverse. Meyer has shown that

$$\frac{1}{n \min_{i \neq 1} |1 - \lambda_i|} \leqslant \max_{1 \leqslant i,j \leqslant n} |Q^{\#}_{i,j}| \leqslant \frac{2(n-1)}{(1-\lambda_2)\ldots(1-\lambda_n)}. \tag{1.1}$$

From these inequalities we see that $Q^{\#}$ furnishes information about the subdominant eigenvalues of A and Meyer goes on to consider the implications that this has to the theory of Markov chains. In the case when Q is symmetric, then $\min(|1-\lambda_i|) = 1-\lambda_2$ and, as $Q^{\#}$ is positive semidefinite, the maximal element in absolute value of $Q^{\#}$ must occur on the main diagonal. A rearrangement of the inequality (1.1) yields the following *upper bounds* on λ_2:

$$1 - \frac{(1-\lambda_2)\dots(1-\lambda_n)}{2n(n-1)} \geqslant 1 - \frac{1}{n}\frac{1}{\max\limits_{1\leqslant i\leqslant n} Q^{\#}_{i,i}} \geqslant \lambda_2.$$

In this paper we develop lower and upper bounds for the second largest and the smallest eigenvalues, respectively, of a nonnegative symmetric matrix in terms of the group inverse of the associated singular M-matrix. We then apply these results to derive bounds on the second smallest and largest eigenvalues of the Laplacian matrix of a connected graph. We pay special attention to the case when the graph is a tree, giving an explicit formula for the group inverse of the Laplacian together with an interpretation of its entries. In so doing we improve a known bound for the algebraic connectivity of a tree. Our lower bound on λ_2 also allows us to sharpen the upper bound on the middle expression in Meyer's result given in (1.1).

Our starting point is simple. Let A be an $n \times n$ symmetric, irreducible, and nonnegative matrix whose eigenvalues are $\lambda_1 > \lambda_2 \geqslant \ldots \geqslant \lambda_n \geqslant -\lambda_1$. Let $v^{(1)}, \ldots, v^{(n)}$, with $v^{(1)} \gg 0$, be an orthonormal set of eigenvectors of A corresponding to $\lambda_1, \ldots, \lambda_n$, respectively. Put $Q = \lambda_1 I - A$. Then $Q^{\#}$ admits a representation in terms of rank 1 idempotents (see, for example, Ben-Israel and Greville [1] or Campbell and Meyer [3]) as follows:

$$Q^{\#} = \sum_{m=2}^{n} \frac{v^{(m)}(v^{(m)})^T}{\lambda_1 - \lambda_m}.$$

Thus for any $1 \leqslant i \leqslant n$, we have that

$$Q^{\#}_{i,i} = \sum_{m=2}^{n} \frac{(v_i^{(m)})^2}{\lambda_1 - \lambda_m}. \tag{1.2}$$

Our bounds are now derived using the fact that, in these equalities, the smallest and largest denominators occur in the summands involving $\lambda_1 - \lambda_2$ and $\lambda_1 - \lambda_n$, respectively.

The plan of this paper is as follows. In Section 2 we derive our principal bounds in Theorems 2.1 and 2.5. In Theorems 2.7 and 2.8 we characterize the case of equality in some of these bounds. In Section 3 we apply our inequalities to the eigenvalues of Laplacians (see Theorem 3.1) and consider the special case when they arise from tree. We also give an interpretation of the entries of $L^{\#}$ (see Theorem 3.3). As example of two results which we obtain in this section we mention that, first of all, from our results in Section 2 we deduce the following bound on the algebraic connectivity ν of a connected graph $\mathcal{G}$ on n vertices with Laplacian L:

$$\nu \leqslant \frac{n-1}{n} \frac{\lambda_1}{\max\limits_{1\leqslant i\leqslant n} L^{\#}_{i,i}}. \tag{1.3}$$

Next, in the particular case when $\mathcal{G}$ is a tree, we show that this bound is sharper than Fiedler's bound:

$$\nu \leqslant \frac{n}{n-1} \min_{1\leqslant i\leqslant n} L_{i,i}.$$

Moreover, we show that the maximal diagonal entry in $L^{\#}$ always occurs in a position corresponding to a pendant vertex.

2. Main results

As was laid out in Section 1, let A be an $n \times n$ symmetric, irreducible, and nonnegative matrix whose eigenvalues are $\lambda_1 > \lambda_2 \geqslant \ldots \geqslant \lambda_n \geqslant -\lambda_1$. Let $v^{(1)}, \ldots, v^{(n)}$, with $v^{(1)} \gg 0$ be corresponding eigenvectors normalized to form an orthonormal basis. Recall the equality

$$Q^{\#}_{i,i} = \sum_{m=2}^{n} \frac{(v_i^{(m)})^2}{\lambda_1 - \lambda_m},$$

for all $1 \leqslant i \leqslant n$, which we derived from the spectral resolution for the group inverse of the associated M-matrix $Q = \lambda_1 I - A$.

We begin by giving a lower bound on λ_2.

Theorem 2.1. *Suppose that A is an $n\times n$ irreducible, nonnegative, and symmetric matrix with Perron root λ_1 and with eigenvalues*

$$\lambda_1 > \lambda_2 \geqslant \lambda_3 \geqslant \ldots \geqslant \lambda_n \geqslant -\lambda_1,$$

then

$$\mu \geqslant \lambda_2 \geqslant \max\left\{ \lambda_1 - \frac{1 - \max\limits_{1\leqslant i\leqslant n} (v_i^{(1)})^2}{\min\limits_{1\leqslant i\leqslant n} Q^{\#}_{i,i}},\ \lambda_1 - \frac{1 - \min\limits_{1\leqslant i\leqslant n} (v_i^{(1)})^2}{\max\limits_{1\leqslant i\leqslant n} Q^{\#}_{i,i}} \right\}. \tag{2.1}$$

In particular, if A has constant row sum λ_1, then

$$\mu \geqslant \lambda_2 \geqslant \lambda_1 - \frac{n-1}{n} \frac{1}{\max\limits_{1\leqslant i\leqslant n} Q^{\#}_{i,i}}. \tag{2.2}$$

P r o o f. Let $v^{(1)}, \dots, v^{(n)}$ be orthonormal eigenvectors corresponding to $\lambda_1, \dots,$ λ_n, respectively. Then, as $\lambda_1 > \lambda_2 \geqslant \lambda_m$, $m = 3, \dots, n$, we have from (1.2) that:

$$Q^{\#}_{i,i} = \sum_{m=2}^{n} \frac{(v_i^{(m)})^2}{\lambda_1 - \lambda_m} \leqslant \sum_{m=2}^{n} \frac{(v_i^{(m)})^2}{\lambda_1 - \lambda_2} = [1 - (v_i^{(1)})^2] \frac{1}{\lambda_1 - \lambda_2}, \tag{2.3}$$

where the last equality follows from the fact

$$\sum_{m=1}^{n} (v_i^{(m)})^2 = 1.$$

Rearranging the inequality (2.3) we obtain after some simple extremal considerations that the inequality (2.1) holds. In the special case when A has constant row sums, $v_i^{(1)} = 1/\sqrt{n}$ for all $i = 1, \dots, n$, easily yielding (2.2). □

Corollary 2.2. *Suppose that A is an $n \times n$ irreducible, symmetric, nonnegative, stochastic matrix with eigenvalues $1 = \lambda_1 > \lambda_2 \geqslant \ldots \geqslant \lambda_n$. Then*

$$\frac{n-1}{n} \frac{1}{1 - \lambda_2} \geqslant \max_{1 \leqslant i \leqslant n} Q^{\#}_{i,i}. \tag{2.4}$$

P r o o f. This is immediate from (2.2) □

Remark 2.3. We see that in the symmetric case, (2.4) can lead to a much sharper upper bound on the middle expression in Meyer's inequality (1.1).

Remark 2.4. Essentially the same proofs shows that if A is an $n \times n$ normal primitive matrix with row sums λ_1 and eigenvalues $\lambda_1 > |\lambda_2| \geqslant |\lambda_3| \geqslant \ldots \geqslant |\lambda_n|$, then

$$\mu \geqslant |\lambda_2| \geqslant \lambda_1 - \frac{n-1}{n} \frac{1}{\max\limits_{1 \leqslant i \leqslant n} Q^{\#}_{i,i}}. \tag{2.5}$$

We now use similar techniques to derive an upper bound on λ_n:

Theorem 2.5. *Suppose that A is an $n \times n$ irreducible nonnegative symmetric matrix with Perron root λ_1. If its eigenvalues are*

$$\lambda_1 > \lambda_2 \geqslant \lambda_3 \geqslant \ldots \geqslant \lambda_n \geqslant -\lambda_1,$$

then

$$\lambda_n \leqslant \min \left\{ \lambda_1 - \frac{1 - \max\limits_{1 \leqslant i \leqslant n} (v_i^{(1)})^2}{\min\limits_{1 \leqslant i \leqslant n} Q^{\#}_{i,i}},\ \lambda_1 - \frac{1 - \min\limits_{1 \leqslant i \leqslant n} (v_i^{(1)})^2}{\max\limits_{1 \leqslant i \leqslant n} Q^{\#}_{i,i}} \right\}. \tag{2.6}$$

In particular, if A also has constant row sums equal to λ_1, then

$$\lambda_n \leqslant \lambda_1 - \frac{n-1}{n} \frac{1}{\min\limits_{1 \leqslant i \leqslant n} Q^{\#}_{i,i}}. \tag{2.7}$$

Proof. As in the proof of Theorem 2.1,

$$Q^{\#}_{i,i} = \sum_{m=2}^{n} \frac{(v_i^{(m)})^2}{\lambda_1 - \lambda_m} \geqslant \frac{1}{\lambda_1 - \lambda_n} \sum_{m=2}^{n} (v_i^{(m)})^2 = [1 - (v_i^{(1)})^2] \frac{1}{\lambda_1 - \lambda_n}.$$

The inequality (2.6) now follows after some algebraic manipulations and simple extremal considerations. The inequality (2.7) for the case in which A has constant row sums follows now because $v_i^{(1)} = 1/\sqrt{n}$ for all $i = 1, \ldots, n$. □

From Meyer [6] we know that the diagonal entries of $Q^{\#}$, $Q = \lambda_1 I - A$, are positive for any irreducible nonnegative matrix A whose Perron root is λ_1. Our next result gives a lower bound on the diagonal entries in the symmetric case. Its proof follows directly from Theorem 2.5 and the fact that $\lambda_n \geqslant -\lambda_1$.

Corollary 2.6. *If A is an $n \times n$ symmetric, irreducible, and nonnegative matrix with Perron root λ_1 and Perron vector $v^{(1)}$ normalized so that $\|v^{(1)}\|_2 = 1$, then*

$$Q^{\#}_{i,i} \geqslant \frac{1 - \max\limits_{1 \leqslant i \leqslant n} (v_i^{(1)})^2}{2\lambda_1}, \quad i = 1, \ldots, n. \tag{2.8}$$

In particular, if A also has constant row sums, then

$$Q^{\#}_{i,i} \geqslant \frac{n-1}{2\lambda_1 n}, \quad i = 1, \ldots, n.$$

Next we characterize the matrices yielding equality between λ_2 and the second expression in the braces of (2.1) in Theorem 2.1:

Theorem 2.7. *Suppose that A is an $n \times n$ irreducible nonnegative symmetric matrix whose Perron root λ_1. If its eigenvalues are $\lambda_1 > \lambda_2 \geqslant \ldots \geqslant \lambda_n \geqslant -\lambda_1$, then*

$$\lambda_2 = \lambda_1 - \frac{1 - \min\limits_{1 \leqslant i \leqslant n} (v_i^{(1)})^2}{\max\limits_{1 \leqslant i \leqslant n} Q^{\#}_{i,i}} \tag{2.9}$$

if and only if there is a permutation matrix P such that

$$P^T AP = \lambda_1 \begin{bmatrix} 1 - x^T x/\alpha & x^T \\ x & (1-\alpha)Y \end{bmatrix}, \tag{2.10}$$

where

$$Yx = x, \tag{2.11}$$

$$x \geqslant \alpha e, \tag{2.12}$$

and

$$1 - \alpha - \frac{x^T x}{\alpha} \geqslant (1-\alpha)\gamma_2, \tag{2.13}$$

where the eigenvalues of Y are $1 = \gamma_1 \geqslant \gamma_2 \ldots \geqslant \gamma_{n-1}$.

P r o o f. Throughout the proof we will suppose, without loss of generality, that $\lambda_1 = 1$ since if this is not the case, we can work with the matrix $A' = (1/\lambda_1)A$. Note that then (2.9) holds if and only if

$$\frac{\lambda_2}{\lambda_1} = 1 - \frac{1 - \min\limits_{1\leqslant i\leqslant n} (v_i^{(1)})^2}{\max\limits_{1\leqslant i\leqslant n} (Q')^{\#}_{i,i}}, \tag{2.14}$$

where $Q' = I - A'$. Consequently, we shall suppose first that equality (2.14) holds and that $\lambda_2 = \lambda_3 = \ldots = \lambda_{j+1} > \lambda_{j+2} \geqslant \ldots \geqslant \lambda_n$ so that λ_2 has multiplicity j. Without loss of generality assume that the maximal diagonal entry in $Q^{\#}$ occurs in its first diagonal position. This is only possible if $v_1^{(m)} = 0$, $j+2 \leqslant m \leqslant n$. Write A as

$$A = \lambda_1 \begin{bmatrix} a & x^T \\ x & M \end{bmatrix}. \tag{2.15}$$

From now on, for an n-vector y, we shall denote by $\bar{y}$ the $(n-1)$-vector obtained by deleting the 1-st entry of y. We next observe that A has at least $j-1$ linearly independent eigenvectors $w^{(1)}, \ldots, w^{(j-1)}$ corresponding to λ_2 whose first entry is 0. To see this, consider any maximally linearly independent set of eigenvectors of A corresponding to λ_2 whose first entry is not 0. Normalize these eigenvectors so that their first entry is 1. If there are k such vectors, then by forming differences we can construct from these $k-1$ linearly independent eigenvectors whose first entry is 0.

Because of the above we find that, necessarily, each of $\overline{w^{(1)}}, \ldots, \overline{w^{(j-1)}}$ is an eigenvector of M corresponding to λ_2 and that each of $\overline{v^{(j+2)}}, \ldots, \overline{v^{(n)}}$ is an eigenvector of M corresponding to $\lambda_{j+2}, \ldots, \lambda_n$, respectively. Moreover, since the first entry in each of $w^{(1)}, \ldots, w^{(j-1)}; v^{(j+2)}, \ldots, v^{(n)}$ is zero and all are eigenvectors of A, it is easy to ascertain from the eigenvalue-eigenvector relation that x is orthogonal to each of their $(n-1)$-dimensional truncations. Hence x is necessarily a nonnegative eigenvector of M corresponding, say, to the eigenvalue $(1-\alpha)$. Notice that since A is irreducible and M is a principal submatrix, $1 > \varrho(M) \geqslant 1-\alpha$ so that $\alpha > 0$.

We next show that for some nonzero scalar β, yet to be determined, the n-vector $(\beta, x^T)^T$ must be a Perron eigenvector of A. From the partitioning of A and the requirement of the eigenvalue-eigenvector relation, we see that $(\beta, x^T)^T$ is an eigenvalue of A if and only if

$$\beta^2 + (1-\alpha-a)\beta - x^T x = 0$$

and the corresponding eigenvalue is $\beta + 1 - \alpha$. Viewing this as a quadratic in β, we find that the equation has 2 distinct real roots:

$$\beta_{1,2} = \frac{a-(1-\alpha) \pm \sqrt{(1-\alpha-a)^2 + 4x^T x}}{2}.$$

Previously we have accounted for $n-2$ linearly independent eigenvectors of A, none of which corresponded to its Perron root. Thus, if β_1 is the positive root of this quadratic, then, necessarily, (β_1, x^T) is, up to a positive multiple, the Perron vector for A corresponding to the Perron root

$$\frac{a-(1-\alpha) + \sqrt{(1-\alpha-a)^2 + 4x^T x}}{2}.$$

(We remark that this shows that the vector x is positive rather than just nonzero nonnegative as we have established earlier, so that, as it is an eigenvector of M corresponding to a nonnegative eigenvalue, it must be a Perron vector of M.) Recalling that the Perron root of A is 1, we see that

$$a = 1 - \frac{x^T x}{\alpha}.$$

Further, since β_2 is not zero, necessarily the eigenvalue corresponding to the eigenvector $(\beta_2, x^T)^T$ is

$$\lambda_2 = 1 - \alpha - \frac{x^T x}{\alpha}.$$

Thus we have established the partitioned form (2.10) of the matrix A and the fact that if Y has eigenvalues $1 \geqslant \gamma_2 \geqslant \ldots \geqslant \gamma_{n-1}$, then necessarily

$$1-\alpha-\frac{x^Tx}{\alpha} \geqslant (1-\alpha)\gamma_2,$$

which is (2.13).

Continuing, it can be checked that the matrix

$$\begin{bmatrix} \alpha x^Tx/(\alpha^2+x^Tx)^2 & -\alpha^2/(\alpha^2+x^Tx)^2x^T \\ -\alpha^2/(\alpha^2+x^Tx)^2x & [I-(1-\alpha)Y]^{-1}-(2\alpha^2+x^Tx)xx^T/[\alpha(\alpha^2+x^Tx)^2] \end{bmatrix}$$

is, precisely, $Q^\#$, and, by our hypothesis,

$$\max_{\lambda_1 \leqslant i \leqslant n} Q^\#_{i,i} = Q^\#_{1,1} = \frac{\alpha x^Tx}{(\alpha^2+x^Tx)^2}.$$

Also, it is readily verified that $\beta_1 = \alpha$, so that

$$v^{(1)} = \frac{1}{\sqrt{\alpha^2+x^Tx}}\begin{pmatrix}\alpha \\ x\end{pmatrix}$$

is the Perron vector of A normalized so that $\|v^{(1)}\|_2 = 1$.

Since

$$\lambda_2 = 1-\alpha-\frac{x^Tx}{\alpha} = 1-\left(\frac{1-\min\limits_{1\leqslant i\leqslant n}(v_i^{(1)})^2}{\max\limits_{1\leqslant i\leqslant n} Q^\#_{i,i}}\right),$$

we see that, in fact,

$$\min_{1\leqslant i\leqslant n}(v_i^{(1)})^2 = \frac{\alpha^2}{\alpha^2+x^Tx},$$

so that $x_i \geqslant \alpha$, for all $1 \leqslant i \leqslant n$. Hence $x \geqslant \alpha e$, and the remaining necessary condition (2.12) has been established.

Now suppose that A is of the form stated in the theorem. As above, we see that

$$\lambda_2 = 1-\alpha-\frac{x^Tx}{\alpha},$$

that

$$\min_{1\leqslant i\leqslant n}(v_i^{(1)}) = \frac{\alpha^2}{\alpha^2+x^Tx},$$

and that

$$Q^\# = \begin{bmatrix} \alpha x^Tx/(\alpha^2+x^Tx)^2 & -\alpha^2/(\alpha^2+x^Tx)^2x^T \\ -\alpha^2/(\alpha^2+x^Tx)^2x & [I-(1-\alpha)Y]^{-1}-(2\alpha^2+x^Tx)xx^T/[\alpha(\alpha^2+x^Tx)^2] \end{bmatrix}.$$

Thus our proof will be done provided we can show that

$$\max_{1\leqslant i\leqslant n} Q^{\#}_{i,i} = \frac{\alpha x^T x}{(\alpha^2 + x^T x)^2}.$$

For this purpose let $z^{(2)}, \ldots, z^{(n)}$ be an orthonormal set of eigenvectors of Y corresponding to $\gamma_2, \ldots, \gamma_n$, respectively. Then we see that for each $1 \leqslant i \leqslant n-1$,

$$\begin{aligned}[I-(1-\alpha)Y]^{-1}_{i,i} &= \frac{1}{\alpha}\frac{x_i^2}{x^T x} + \sum_{m=2}^{n-1} \frac{1}{1-(1-\alpha)\gamma_m}(z_i^{(m)})^2 \\ &\leqslant \frac{1}{\alpha}\frac{x_i^2}{x^T x} + \frac{1}{1-(1-\alpha)\gamma_2}\Big(1-\frac{x_i^2}{x^T x}\Big).\end{aligned}$$

Hence

$$\begin{aligned}&[I-(1-\alpha)Y]^{-1}_{i,i} - (2\alpha^2 + x^T x)x_i^2/[\alpha(\alpha^2+x^T x)^2] \\ &\qquad\leqslant \frac{1}{\alpha}\frac{x_i^2}{x^T x} + \frac{\alpha}{\alpha^2 + x^T x}\Big(1-\frac{x_i^2}{x^T x}\Big) - (2\alpha^2 + x^T x)x_i^2/[\alpha(\alpha^2+x^T x)^2] \\ &\qquad= \frac{\alpha}{\alpha^2+x^T x} - (2\alpha^2 + x^T x)x_i^2/[\alpha(\alpha^2+x^T x)^2] \\ &\qquad\leqslant \frac{\alpha x^T x}{(\alpha^2+x^T x)^2},\end{aligned}$$

the last inequality following from (2.12), and so

$$\max_{1\leqslant i\leqslant n} Q^{\#}_{i,i} = \frac{\alpha x^t x}{(\alpha^2 + x^T x)^2},$$

as desired. □

In our next result we consider the case of equality in the inequality between λ_n and the first expression in the braces of (2.6) in part of Theorem 2.5. The proof is analogous to that of Theorem 2.7.

Theorem 2.8. *Suppose A is an $n\times n$ symmetric, irreducible, and nonnegative matrix whose Perron root is λ_1. If the eigenvalues of A are $\lambda_1 > \lambda_2 \geqslant \ldots \geqslant \lambda_n \geqslant -\lambda_1$, then*

$$\lambda_n = \lambda_1 - \frac{1 - \max\limits_{1\leqslant i\leqslant n}(v_i^{(1)})^2}{\min\limits_{1\leqslant i\leqslant n} Q^{\#}_{i,i}} \tag{2.16}$$

if and only if there exists a permutation matrix P such that

$$P^T AP = \lambda_1 \begin{bmatrix} 1 - x^T x/\alpha & x^T \\ x & (1-\alpha)Y \end{bmatrix}, \tag{2.17}$$

where $x \gg 0$, $\alpha \geqslant 0$,

$$Yx = x,$$

$$x \leqslant \alpha e,$$

and

$$1 - \alpha - \frac{x^T x}{\alpha} \leqslant (1-\alpha)\gamma_{n-1}, \tag{2.18}$$

where the eigenvalues of Y are $1 = \gamma_1 \geqslant \gamma_2 \geqslant \gamma_{n-1}$.

Corollary 2.9. *From Corollary 2.6, we have that if A is an $n \times n$ symmetric, irreducible, and nonnegative matrix with Perron root λ_1, then*

$$\min_{1\leqslant i\leqslant n} Q^{\#}_{i,i} \geqslant \frac{1 - \max\limits_{1\leqslant i\leqslant n} (v_i^{(1)})^2}{2\lambda_1}. \tag{2.19}$$

Equality holds if and only if there is a permutation matrix P such that

$$P^T AP = \lambda_1 \begin{bmatrix} a & x^T \\ x & M \end{bmatrix}, \tag{2.20}$$

where $x^T x = 1$.

Proof. As in the proof of Theorem 2.7 we can suppose that $\lambda_1 = 1$. Assume now that equality holds in (2.19). Then from (2.16) we easily deduce that $\lambda_n = -1$ and so λ_n also satisfies (2.6). Hence by Theorem 2.7, there exists a permutation matrix P such that

$$P^T AP = \begin{bmatrix} 1 - x^T x & x^T \\ x & (1-\alpha)Y \end{bmatrix},$$

for some positive scalar $\alpha \leqslant 1$ and a positive vector x such that $Yx = x$. Since A is irreducible, but has an eigenvalue -1 as well as 1, the latter being its spectral radius, A must by 2-cyclic, and so, e.g. Varga [15] or Berman and Plemmons [2], A must have zero diagonal entries showing that $x^T x/\alpha = 1$. As in the proof of Theorem 2.7 where it was shown that (under the conditions of the Theorem 2.8) $\lambda_2 = 1 - \alpha - x^T x/\alpha$, so too in the proof of Theorem 2.8 it is established that (under the conditions of that theorem) $\lambda_n = 1 - \alpha - x^T x/\alpha$. Thus, as $\lambda_n = -1$, we can now conclude that $\alpha = 1$. Whence $x^T x = 1$ and $P^T AP$ must have the desired form of (2.20).

Conversely, suppose without loss of generality that A is already in the form given in (2.20) with $x^T x = 1$. Then

$$Q^{\#} = \begin{bmatrix} 1/4 & -(1/4)x^T \\ -(1/4)x & I - (3/4)x^T x \end{bmatrix}.$$

Also, it is easily verified that

$$v^{(1)} = \frac{\lambda_1}{\sqrt{2}} \begin{pmatrix} \lambda_1 \\ x \end{pmatrix}.$$

Whence,

$$\frac{\lambda_1}{4} = \min_{1 \leqslant i \leqslant n} Q^{\#}_{i,i} = \frac{1 - 1/2}{2} = \frac{1 - \max\limits_{\lambda_1 \leqslant i \leqslant n} (v_i^{(1)})^2}{2},$$

completing our proof. □

3. Applications

We now apply the results of the previous section to obtain bounds on the algebraic connectivity and the largest eigenvalue of a connected graph.

Theorem 3.1. *Suppose $\mathcal{G}$ is a connected graph on n vertices with Laplacian matrix L. Then the algebraic connectivity, ν, of G satisfies*

$$\nu \leqslant \frac{n-1}{n} \frac{1}{\max\limits_{1 \leqslant i \leqslant n} L^{\#}_{i,i}} \tag{3.1}$$

and the largest eigenvalue, β, of L satisfies that

$$\beta \geqslant \frac{n-1}{n} \frac{1}{\min\limits_{1 \leqslant i \leqslant n} L^{\#}_{i,i}}. \tag{3.2}$$

Equality in (3.1) *holds if and only if $\mathcal{G}$ is the complete graph.*

Proof. Let d denote the largest degree of a vertex of G. Then L can be written as

$$L = d(I - M) \tag{3.3}$$

where M is an irreducible, nonnegative, symmetric and stochastic matrix. Clearly, by (3.3),

$$L^{\#} = \frac{1}{d}(I - M)^{\#} =: Q^{\#}.$$

Letting the eigenvalues of M be $1 = \lambda_1 > \lambda_2 \geqslant \ldots \geqslant \lambda_n$, we see that $\nu = d(1 - \lambda_2)$ and $\beta = d(1 - \lambda_n)$. The inequality in (3.1) now follows from (2.1) of Theorem 2.1, and that in (3.2) follows from (2.7) of Theorem 2.5.

A straightforward computation shows that if G is the complete graph, the equality holds in (3.1).

Now assume that equality holds in (3.1). Then λ_2 equals the second expression in the braces on the righthand side of (2.1). Thus, by Theorem 2.7, we may assume without loss of generality that

$$M = \begin{bmatrix} 1 - x^T x/\alpha & x^T \\ x & (1-\alpha)Y \end{bmatrix},$$

for some nonnegative α, x and Y satisfying (2.11), (2.12) and (2.13), where the eigenvalues of Y are $1 = \gamma_1 > \gamma_2 \geqslant \ldots \geqslant \gamma_{n-1}$. Since the off-diagonal entries of L agree with those of $-dM$, and each off-diagonal entry of L is either 0 or -1, it follows from (2.12) that vertex 1 of G has degree $n-1$, $d = n-1$ and

$$x = \frac{1}{n-1}e.$$

Thus, since $x \geqslant \alpha e$, $\frac{1}{n-1} \geqslant \alpha$. The $(1,1)$-entry of M is nonnegative and equals

$$1 - xx^T/\alpha = 1 - \frac{1}{(n-1)\alpha}.$$

Thus $\alpha \geqslant \frac{1}{n-1}$. We conclude that $\alpha = \frac{1}{n-1}$. Substituting $\alpha = \frac{1}{n-1}$ into (2.13) and simplifying yields that

$$\gamma_2 \leqslant -\frac{1}{n-2}.$$

Thus we can write that

$$0 \leqslant \text{trace}(Y) = 1 + \sum_{j=2}^{n-1} \gamma_j \leqslant 1 + (n-2)\gamma_2 \leqslant 0,$$

which shows that $\text{trace}(Y) = 0$. As Y is a nonnegative matrix, its entire diagonal is 0 implying that each diagonal entry of L equals $n-1$. This shows that the degree of each vertex in $\mathcal{G}$ is $n-1$ and hence $\mathcal{G}$ is the complete graph (on n vertices). $\square$

The following example shows that while equality in (3.1) can hold only for a complete graph, (3.1) can still yield a good bound for other graphs.

Example 3.2. The *star on $n \geqslant 2$ vertices* has an adjacency matrix

$$A = \begin{bmatrix} 0 & e^T \\ e & O \end{bmatrix}$$

and Laplacian

$$L = \begin{bmatrix} (n-1) & -\,e^T \\ -\,e & I \end{bmatrix}.$$

The eigenvalues of L are easily computed to be 0, $\nu = 1$, and $\beta = n$, and

$$L^{\#} = \begin{bmatrix} (n-1)/n^2 & -\,(1/n^2)e^T \\ -\,(1/n^2)e & I - [(n+1)/n^2]J \end{bmatrix}.$$

Thus

$$\max_{1 \leqslant i \leqslant n} L^{\#}_{i,i} = \frac{n^2 - n - 1}{n^2},$$

so that

$$\frac{n-1}{n} \frac{1}{\max\limits_{1 \leqslant i \leqslant n} L^{\#}_{i,i}} = \frac{n^2 - n}{n^2 - n - 1} = 1 + \frac{1}{n^2 - n + 1}.$$

Therefore, the bound in (3.1) differs from the true value of ν by $1/(n^2 - n - 1)$. This difference obviously tends to 0 as n tends to ∞.

We also note that for the star

$$\min_{1 \leqslant i \leqslant n} L^{\#}_{i,i} = \frac{n-1}{n^2},$$

so that

$$\frac{n-1}{n} \frac{1}{\min\limits_{1 \leqslant i \leqslant n} L^{\#}_{i,i}} = n = \beta.$$

Thus the star provides an example of a graph for which equality in (3.2) holds.

Theorem 2.1 illustrates that the entries of the group inverse $L^{\#}$ of the Laplacian L of a graph are related to the algebraic connectivity of G. We now present a combinatorial interpretation of the entries of $L^{\#}$ in the case that G is a tree. Let T be a tree with vertices $1, 2, \ldots, n$, and with Laplacian L. Since T is a tree there is a unique path of T joining any two vertices of T. For vertices i and j we let $[i, j)$ denote the set of vertices $k \neq j$ which lie on the path from i to j. The number of vertices k for which the path in T from k to j contains i is denoted by $b_j(i)$ and is called the *bottleneck number for i with terminal vertex j*. The following theorem describes the entries of $L^{\#}$ in terms of the bottleneck numbers with a fixed terminal vertex.

Theorem 3.3. *Suppose T is a tree with vertices $1, 2, \ldots, n$ and Laplacian L. Then*

$$L^{\#}_{i,j} = \begin{cases} |[i,n) \cap [j,n)| - \sum\limits_{k \in [i,n)} \frac{b_n(k)}{n} \\ \qquad - \sum\limits_{k \in [j,n)} \frac{b_n(k)}{n} + \sum\limits_{k=1}^{n-1} \frac{b_n(k)^2}{n^2} & \text{if} \quad i \neq n \quad \text{and} \quad j \neq n, \\ - \sum\limits_{k \in [i,n)} \frac{b_n(k)}{n} + \sum\limits_{k=1}^{n-1} \frac{b_n(k)^2}{n^2} & \text{if} \quad i \neq n \quad \text{and} \quad j = n, \\ - \sum\limits_{k \in [j,n)} \frac{b_n(k)}{n} + \sum\limits_{k=1}^{n-1} \frac{b_n(k)^2}{n^2} & \text{if} \quad i = n \quad \text{and} \quad j \neq n, \\ \sum\limits_{k=1}^{n-1} \frac{b_n(k)^2}{n^2} & \text{if} \quad i = n \quad \text{and} \quad j = n. \end{cases}$$

P r o o f. Since T is a tree, we may relabel the vertices $1, 2, \ldots, n-1$, so that the vertices along each path of T beginning with n are in decreasing order. Furthermore, since T is a tree, after such a relabeling for each vertex $j \neq n$, there exists a unique edge e_j of the form $\{j, i\}$ such that $i > j$. Clearly $e_j \neq e_k$ if $k \neq j$. Thus, since T has $n-1$ edges, the edges of T are precisely $e_1, e_2, \ldots, e_{n-1}$. Let $B = [b_{ij}]$ be the n by $n-1$ oriented incidence matrix of T defined by

$$b_{ij} = \begin{cases} -1 & \text{if } e_j = \{i, j\}, \\ 1 & \text{if } i = j, \\ 0 & \text{otherwise.} \end{cases}$$

Then $L = BB^T$ as in [4]. Since each column sum of B is 0, we may write that

$$B = \begin{bmatrix} \widehat{B} \\ -e^T \widehat{B} \end{bmatrix},$$

where $\widehat{B}$ is an $n-1$ by $n-1$ matrix. Since L has rank $n-1$, $\widehat{B}$ is invertible, and $L = BB^T$ is a full rank factorization of L. Hence, $L^{\#} = B(BB^T)^{-2}B^T$. Using the partitioned form of B, a straightforward calculation yields that

$$L^{\#} = \begin{bmatrix} U & V \\ V^T & W \end{bmatrix}, \tag{3.4}$$

where

$$\begin{aligned}
U &= (\widehat{B})^{-T}(\widehat{B})^{-1} - \frac{1}{n}(\widehat{B})^{-T}(\widehat{B})^{-1}ee^T \\
&\quad - \frac{1}{n}ee^T(\widehat{B})^{-T}(\widehat{B})^{-1} + \frac{e^T(\widehat{B})^{-T}(\widehat{B})^{-1}e}{n^2}ee^T, \\
V &= -\frac{1}{n}(\widehat{B})^{-T}(\widehat{B})^{-1}e + \frac{e^T(\widehat{B})^{-T}(\widehat{B})^{-1}e}{n^2}e, \\
W &= \frac{e^T(\widehat{B})^{-T}(\widehat{B})^{-1}e}{n^2}.
\end{aligned}$$

Note by the assumptions on the labeling of the edges of T and of the vertices $1, 2, \ldots, n-1$ of T,

$$\widehat{B} = I - N,$$

where $N = [n_{ij}]$ is the strictly lower triangular $(0,1)$-matrix of order $n-1$ with $n_{ij} = 1$ if and only if $i > j$ and $\{i, j\}$ is an edge of T. It follows that for any nonnegative integer k and for $i, j \in \{1, 2, \ldots, n-1\}$, the (i,j)-entry of N^k equals the number of paths in T of length k from j to i such that the vertices along the path are in increasing order. Let $j = v_0,\ v_1, \ldots, v_\ell = n$ be the path from j to n. Since for each vertex $k \neq n$ of T there exists a unique edge in T of the form $\{k, \ell\}$ where $k < \ell$, every path whose initial vertex is j and whose vertices along the path are in increasing order is necessarily a subpath of the path from j to n. Thus, the (i,j)-entry of N^k equals 1 if and only if $k \leqslant \ell - 1$ and $i = v_k$. Clearly, since N is strictly lower triangular and $\widehat{B} = I - N$,

$$\widehat{B}^{-1} = \sum_{k=0}^{n-2} N^k.$$

Hence the (i,j)-entry of $\widehat{B}^{-1}$ equals 1 if $i \in [j, n)$ and equals 0 otherwise. The entries of $M := \widehat{B}^{-T}\widehat{B}^{-1}$ are the inner products of the columns of $\widehat{B}^{-1}$, and hence the (i,j)-entry of M equals $|[i,n) \cap [j,n)|$. The ith entry of Me equals

$$\sum_{j=1}^{n-1}(|[i,n) \cap [j,n)|).$$

For each $k \in [i,n)$, there exist exactly $b_n(k)$ vertices j such that $k \in [j,n)$. Therefore, the ith entry of Me equals

$$\sum_{k \in [i,n)} b_n(k).$$

This implies that

$$e^T M e = \sum_{i=1}^{n-1} \sum_{k \in [i,n)} b_n(k). \tag{3.5}$$

For each $k \in \{1, 2, \ldots, n-1\}$, the term $b_n(k)$ occurs as a summand in (3.5) exactly $b_n(k)$ times. Thus,

$$e^T M e = \sum_{i=1}^{n} b_n(k)^2.$$

The theorem now follows from (3.4). □

Remark 3.4. In Fiedler [4] it is shown that if L is the Laplacian of a graph $\mathcal{G}$ on n vertices, then

$$\nu \leqslant \frac{n}{n-1} \min_{1 \leqslant i \leqslant n} L_{i,i}. \tag{3.6}$$

It is reasonable to compare the tightness of the upper bound on ν given by our bound (3.1) with the Fiedler's bound (3.6). For any tree $\mathcal{G}$ with 3 or more vertices, (3.1) is better than (3.6). This can be seen as follows. Let T be a tree on $n \geqslant 3$ vertices, and assume that vertex n is a pendant vertex of T. Let j be the unique vertex of T which is adjacent to n. Then $b_n(j) = n-1$, and $b_n(i) > 0$ for each vertex $i \neq j, n$. Hence by Theorem 3.3, $L^{\#}_{n,n} > \frac{(n-1)^2}{n^2}$. This implies that

$$\frac{n-1}{n} \frac{1}{\max\limits_{1 \leqslant i \leqslant n} L^{\#}_{i,i}} \leqslant \frac{n}{n-1}.$$

Since for a tree $\min\limits_{1 \leqslant i \leqslant n} L_{ii} = 1$, the result follows.

We now show that the maximum diagonal entry of the group inverse of the Laplacian of a tree occurs at a position corresponding to a pendant vertex.

Theorem 3.5. *Let T be a tree with vertices $1, 2, \ldots, n$ and with Laplacian L. Let j be vertex of T such that $L^{\#}_{j,j} = \max\limits_{1 \leqslant i \leqslant n} L^{\#}_{i,i}$. Then j is a pendant vertex of T.*

Proof. Consider a vertex i which is adjacent to j. Then $[j, i)$ contains only vertex j. Hence the formula for $L^{\#}_{j,j}$ in Theorem 3.3, with n taken to be i, simplifies to

$$L^{\#}_{j,j} = 1 - \frac{2b_i(j)}{n} + \sum_{k \neq i} \frac{b_i(k)^2}{n^2}.$$

Hence, by the formula for $L^{\#}_{n,n}$ in Theorem 3.3,

$$L^{\#}_{j,j} - L^{\#}_{i,i} = 1 - \frac{2b_i(j)}{n}.$$

By assumption $L^{\#}_{j,j} \geqslant L^{\#}_{i,i}$, and thus the previous equality implies that

$$\frac{n}{2} \geqslant b_i(j)$$

for all vertices i adjacent to j. Let $i_1, i_2, \ldots, i_\ell$ be the vertices of T adjacent to j. Then

$$\frac{\ell n}{2} \geqslant \sum_{k=1}^{\ell} b_{i_k}(j).$$

For vertex j, each of the vertices i_k has the property that the path from j to i_k contains j. For each vertex v of T other than j, exactly $\ell - 1$ of the vertices i_k have the property that the path from v to i_k contains j. Thus vertex j contributes exactly ℓ and each other vertex of T contributes exactly $\ell - 1$ to the righthand side of the above equation. Hence,

$$\frac{\ell n}{2} \geqslant (\ell - 1)(n - 1) + \ell,$$

from which it easily follows that $\ell \leqslant 1$. Hence vertex j is a pendant vertex. $\square$

Example 3.6. For a graph G with vertices $1, 2, \ldots, n$, the *Wiener index* is

$$w(G) := \sum_{i<j} d(i, j),$$

where $d(i, j)$ is the distance between vertex i and j in G. Thus if G is a tree, $d(i, j) = |[i, j)|$. The following is a standard theorem (see, for example, [11]).

Let T be a tree on n vertices whose Laplacian has eigenvalues

$$\mu_1 = 0 < \mu_2 \leqslant \mu_3 \leqslant \ldots \leqslant \mu_n,$$

then

$$w(T) = \sum_{i=2}^{n} \frac{n}{\mu_i}.$$

This theorem can be proven using our combinatorial description of the entries of the group inverse of the Laplacian of a tree as follows. First note that the nonzero eigenvalues of $L^{\#}$ are $1/\mu_2, \ldots, 1/\mu_n$, and hence

$$n \operatorname{trace}(L^{\#}) = \sum_{i=2}^{n} \frac{n}{\mu_i}.$$

For each i and j, Theorem 3.3 implies that

$$2L^{\#}_{i,i} = |[i,j)| - 2\sum_{k\in[i,j)} \frac{b_j(k)}{n} + \sum_{k:k\neq j} \frac{b_j(k)^2}{n^2} + \sum_{k:k\neq i}^{n} \frac{b_i(k)^2}{n^2}. \tag{3.7}$$

Summing equation (3.7) over all i and j yields that

$$\begin{aligned} 2\sum_{i,j=1}^{n} L^{\#}_{i,i} = {} & \sum_{i,j=1}^{n} |[i,j)| - 2\sum_{i,j=1}^{n}\sum_{k\in[i,j)} \frac{b_j(k)}{n} \\ & + n\sum_{j=1}^{n}\sum_{k\neq j} \frac{b_j(k)^2}{n^2} + n\sum_{i=1}^{n}\sum_{k\neq i} \frac{b_i(k)^2}{n^2}. \end{aligned} \tag{3.8}$$

The lefthand side of (3.8), simplifies to $2n$ trace$(L^{\#})$. The first summand on the righthand side simplifies to $2\sum\limits_{i<j} d(i,j)$. Each $b_j(k)$ with $j \neq k$ occurs $b_j(k)$ times in the second term in (3.8). Hence this second term simplifies to

$$-\frac{2}{n}\sum_{k,j:k\neq j} b_j(k)^2,$$

which is precisely the sum of the last two sums in (3.8). Therefore,

$$2n \text{ trace}(L^{\#}) = 2\sum_{i<j} d(i,j).$$

This along with (3.5), imply that $\sum\limits_{i=2}^{n} \frac{n}{\mu_i} = w(T)$.

Theorem 3.7. *Let T be a tree on $n \geqslant 2$ vertices with Laplacian L. Let d be the maximum degree of a vertex of T. Then $L^{\#}_{i,i} \geqslant \frac{(n-1)^2}{n^2}$ for some i, and*

$$L^{\#}_{i,i} \geqslant \frac{(n-1)^2}{dn^2}$$

for all i.

P r o o f. We have already see in Remark 3.4, that if i is a pendant vertex, then $L^{\#}_{i,i} \geqslant \frac{(n-1)^2}{n^2}$. Let i be a vertex and let the vertices adjacent to i be $j_1, j_2, \ldots, j_\ell$. Then by Theorem 3.3,

$$L^{\#}_{i,i} \geqslant \frac{1}{n^2}\sum_{k=1}^{\ell} b_i(j_k)^2.$$

It is easily seen that $\sum\limits_{k=1}^{\ell} b_i(j_k) = n-1$. Hence, by the Cauchy-Schwarz inequality, $\sum\limits_{k=1}^{\ell} b_i(j_k)^2 \geqslant \frac{(n-1)^2}{\ell}$. It follows that $L^{\#}_{i,i} \geqslant \frac{(n-1)^2}{dn^2}$. □

Note that Theorem 3.3 implies that $L^{\#}_{i,i} \geqslant \frac{n-1}{n^2}$ with equality only if i is the center vertex of a star. It is easy to verify that if i is the center vertex of the star, then equality does in fact hold.

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