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Optimizing quadratic forms of adjacency matrices of trees and related eigenvalue problems

Wai-Shun Cheung [a], Chi-Kwong Li [b,1], D.D. Olesky [c,*,2], P. van den Driessche [a,2]

[a] *Department of Mathematics and Statistics, University of Victoria, Victoria, BC, Canada V8W 3P4*
[b] *Department of Mathematics, College of William and Mary, Williamsburg, VA 23187, USA*
[c] *Department of Computer Science, University of Victoria, Victoria, BC, Canada V8W 3P6*

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Abstract

Let A be an adjacency matrix of a tree T with n vertices. Conditions are determined for the existence of a fixed permutation matrix P that maximizes the quadratic form $x^t P^t A P x$ over all nonnegative vectors x with entries arranged in nondecreasing order. This quadratic form problem is completely solved, and its answer leads to a corresponding solution for the problem of determining conditions for the existence of a fixed permutation matrix P that maximizes the largest eigenvalue of matrices of the form $PDP^t + A$, over all real diagonal matrices D with nondecreasing diagonal entries. It is shown that there is a tree with six vertices for which neither of the problems has a solution, and all other trees with six or fewer vertices have solutions for both problems. By duality, the results also apply to the analogous problem of minimizing the smallest eigenvalue of matrices of the form $PDP^t + A$. © 2001 Elsevier Science Inc. All rights reserved.

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* Corresponding author.
E-mail addresses: wshun@math.uvic.ca (W.-S. Cheung), ckli@math.wm.edu (C.-K. Li), dolesky@csr.uvic.ca (D.D. Olesky), pvdd@math.uvic.ca (P. van den Driessche).

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PII: S 0 0 2 4 - 3 7 9 5 (0 0) 0 0 3 0 5 - 0

1. Introduction

Let $A = [a_{ij}]$ be an adjacency matrix of a given tree T with $n \geqslant 3$ vertices. Note that A is a symmetric (0, 1) matrix with all $a_{ii} = 0$. Let S_n be the set of $n \times n$ permutation matrices, and let $\mathbb{R}^n_{+\uparrow} = \{x = (x_1, \ldots, x_n)^{\mathrm{t}}\colon\ 0 \leqslant x_1 \leqslant \cdots \leqslant x_n\}$, i.e., the set of nonnegative vectors in $\mathbb{R}^n$ with entries arranged in nondecreasing order. We study the following optimization problem.

Problem 1.1. Given an adjacency matrix A of a tree with n vertices, determine conditions for the existence of $P \in S_n$ such that for all $x \in \mathbb{R}^n_{+\uparrow}$

$$x^{\mathrm{t}} P^{\mathrm{t}} A P x \geqslant x^{\mathrm{t}} Q^{\mathrm{t}} A Q x \quad \forall Q \in S_n, \tag{1}$$

and characterize P if it exists.

We give a complete solution to Problem 1.1, and use it to solve the following related problem, in which we denote the maximum eigenvalue of a real symmetric matrix B by $\lambda_{\max}(B)$.

Problem 1.2. Given an adjacency matrix A of a tree with n vertices, determine conditions for the existence of $P \in S_n$ such that for all $D = \operatorname{diag}(d_1, \ldots, d_n)$ with $d_1 \leqslant \cdots \leqslant d_n$

$$\lambda_{\max}\big(PDP^{\mathrm{t}} + A\big) \geqslant \lambda_{\max}\big(QDQ^{\mathrm{t}} + A\big) \quad \forall Q \in S_n,$$

and characterize P if it exists.

Note that if P exists, then it is independent of the values of d_i. We write the maximum value of $\lambda_{\max}(PDP^{\mathrm{t}} + A)$ for $P \in S_n$ as $\max \lambda_{\max}(PDP^{\mathrm{t}} + A)$. It is sometimes convenient to change the inequality in Problem 1.2 to the equivalent form

$$\lambda_{\max}\big(D + P^{\mathrm{t}} A P\big) \geqslant \lambda_{\max}\big(D + Q^{\mathrm{t}} A Q\big) \quad \forall Q \in S_n,$$

which entails reordering the rows and columns of A or equivalently relabelling the vertices of T.

Special cases of Problem 1.2 have been studied in the literature. Motivated by results concerning nonuniform strings [7] and the Shrödinger operator [1], attention has focussed on matrices of the form $L + D$, where L is the discrete Laplacian, namely, $L = 2I - A$, where A is the (tridiagonal) adjacency matrix of a path graph. Ashbaugh and Benguria [1, (7.1)] found the permutation matrix P that gives $\max \lambda_{\max}(PDP^{\mathrm{t}} + L)$. Since $PDP^{\mathrm{t}} + L$ is similar to $P(D + 2I)P^{\mathrm{t}} + A$ via a signature (diagonal orthogonal) matrix, their problem is basically the same as Problem 1.2, where A is the adjacency matrix of a path. Specifically, they proved [1, (7.1)] the following result where, by the symmetry of a path, there are two solutions, with a maximum d_i placed at a center vertex of the path.

Theorem 1.3. *Let $A = [a_{ij}]$ be the adjacency matrix of a path graph with n vertices, i.e., $a_{ij} = 1$ if $|i - j| = 1$, and 0 otherwise. Then for all $D = \operatorname{diag}(d_1, \ldots, d_n)$ with $d_1 \leqslant \cdots \leqslant d_n$, $\max \lambda_{\max}(PDP^{\mathrm{t}} + A)$ occurs for $P \in S_n$ so that $PDP^{\mathrm{t}} = \operatorname{diag}(d_1, d_3, d_5, \ldots, d_6, d_4, d_2)$ or $\operatorname{diag}(d_2, d_4, d_6, \ldots, d_5, d_3, d_1)$.*

A careful study of the proofs in [1] reveals that the authors actually solve Problem 1.1 on maximizing a quadratic form when A is restricted to be the adjacency matrix of a path. Specifically, we can restate [1, Lemma 2.1] as follows.

Theorem 1.4. *Let $A = [a_{ij}]$ be the adjacency matrix of a path graph with n vertices, i.e., $a_{ij} = 1$ if $|i - j| = 1$, and 0 otherwise. Suppose P is a permutation matrix such that*

$$P^{\mathrm{t}}AP = \begin{bmatrix} 0 & 0 & 1 & & & & & \\ 0 & & & 1 & & & \text{\Large 0} & \\ 1 & & & & \ddots & & & \\ & 1 & & \text{\Large 0} & & & & \\ & & \ddots & & & & & \\ & & & & & & 1 & \\ & & & & & & & 1 \\ & \text{\Large 0} & & & 1 & & & 1 \\ & & & & & 1 & 1 & 0 \end{bmatrix},$$

i.e., the (i, j) entry of $P^{\mathrm{t}}AP$ is 1 if $|i - j| = 2$ or $i + j = 2n - 1$, and 0 otherwise. Then for all $x \in \mathbb{R}^n_{+\uparrow}$

$$x^{\mathrm{t}}P^{\mathrm{t}}APx \geqslant x^{\mathrm{t}}Q^{\mathrm{t}}AQx \quad \forall Q \in S_n.$$

For the path graph, the problem of determining $\max \lambda_{\max}(PDP^{\mathrm{t}} + A)$, where D has exactly one nonzero entry that is equal to a given $t > 0$ was solved in [3]. The method used in [3] relies on results in [6] where this restricted problem was considered for general A, and was shown to be equivalent to determining $\max \lambda_{\max}(PDP^{\mathrm{t}} + A)$, where D is any nonnegative real diagonal matrix with trace $D = t$.

A relation between our two problems is given by the following proposition, from which it follows that if P is a solution to Problem 1.1, then P is a solution to Problem 1.2. The proposition is proved for any nonnegative symmetric matrix, and thus holds in particular for an adjacency matrix A.

Proposition 1.5. *Let B be an irreducible nonnegative symmetric matrix. Suppose $P \in S_n$ is such that for all $x \in \mathbb{R}^n_{+\uparrow}$*

$$x^{\mathrm{t}}P^{\mathrm{t}}BPx \geqslant x^{\mathrm{t}}Q^{\mathrm{t}}BQx \quad \forall Q \in S_n.$$

Then for all $D = \operatorname{diag}(d_1, \ldots, d_n)$ *with* $d_1 \leqslant \cdots \leqslant d_n$

$$\lambda_{\max}\big(PDP^{\mathrm{t}} + B\big) \geqslant \lambda_{\max}\big(Q^{\mathrm{t}}DQ + B\big) \quad \forall Q \in S_n.$$

Proof. The matrix $Q^{\mathrm{t}}DQ + B$ is essentially nonnegative. Thus, for any $Q \in S_n$, by Perron Frobenius and Rayleigh Ritz (see, e.g., [5, Theorems 8.4.4 and 4.2.2]) there is a positive unit eigenvector $x = (x_1, \ldots, x_n)^{\mathrm{t}}$ such that $\lambda_{\max}(Q^{\mathrm{t}}DQ + B) = x^{\mathrm{t}}(Q^{\mathrm{t}}DQ + B)x$. Let $\tilde{x}$ be obtained from x by rearranging its entries in nondecreasing order. Then

$$\begin{aligned} x^{\mathrm{t}}\big(Q^{\mathrm{t}}DQ + B\big)x &\leqslant x^{\mathrm{t}}Q^{\mathrm{t}}DQx + \tilde{x}^{\mathrm{t}}P^{\mathrm{t}}BP\tilde{x} \\ &\leqslant \tilde{x}^{\mathrm{t}}D\tilde{x} + \tilde{x}^{\mathrm{t}}P^{\mathrm{t}}BP\tilde{x} \\ &\leqslant \lambda_{\max}\big(PDP^{\mathrm{t}} + B\big). \end{aligned}$$

The first inequality is from the definition of P, the second from the ordering of the diagonal elements of D, and the third from Rayleigh Ritz. □

In this paper, we give a complete solution for Problem 1.1, which leads (by Proposition 1.5) to a corresponding solution for Problem 1.2. We do not know whether a solution to Problem 1.2 always guarantees a solution to Problem 1.1.

Our paper is organized as follows. In Section 2, we present and prove our main theorem using several lemmas that are of independent interest. In Section 3, we give a characterization of the trees for which there exists a solution to Problem 1.1, and illustrate this with three families of such trees with n vertices. These examples show that every tree with at most five vertices has a solution to both problems, and that for exactly one tree with six vertices there is no solution. Some related results are given in Section 4; these include a duality statement so that our results can be used to solve the dual problem of minimizing the smallest eigenvalue of matrices of the form $PDP^{\mathrm{t}} + A$. Some graph theoretic terms are used in our discussion, and the reader is referred to [2,4] for standard terminology.

2. Optimal permutation matrix

In this section, we prove the following extension of Theorem 1.4, which yields the solution of Problem 1.1. If A is the adjacency matrix of a given tree T, then so is $P^{\mathrm{t}}AP$ for all $P \in S_n$. Therefore, without loss of generality, we can assume that $P = I$. In the following theorem, we solve Problem 1.1 by characterizing the adjacency matrices A such that for all $x \in \mathbb{R}^n_{+\uparrow}$

$$x^{\mathrm{t}}Ax \geqslant x^{\mathrm{t}}Q^{\mathrm{t}}AQx \quad \forall Q \in S_n.$$

Theorem 2.1. *Let A be the adjacency matrix of a tree T with vertices* $\{1, \ldots, n\}$ *labelled according to the row indices of A. Then for all* $x \in \mathbb{R}^n_{+\uparrow}$

$$x^{\mathrm{t}}Ax \geqslant x^{\mathrm{t}}Q^{\mathrm{t}}AQx \quad \forall Q \in S_n, \tag{2}$$

if and only if the following conditions hold:

(I) *The row sums of A, which are the degrees* $d_1, \ldots, d_n$ *of the vertices of T, satisfy* $d_1 \leqslant \cdots \leqslant d_n$.

(II) *If* $A = L + L^{\mathrm{t}}$, *where L is in* (*strictly*) *lower triangular form, then*

$$L = \begin{bmatrix}
\overbrace{0\cdots0}^{d_{r+1}-1} & \overbrace{0\cdots0}^{d_{r+2}-1} & \cdots & \overbrace{0\cdots0}^{d_{n-1}-1} & \overbrace{0\cdots0}^{d_n} & 0\\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0\cdots0 & 0\cdots0 & \cdots & 0\cdots0 & 0\cdots0 & 0\\
1\cdots1 & & & & & 0\\
& 1\cdots1 & & & \text{\Large 0} & 0\\
& & \ddots & & & \vdots\\
& \text{\Large 0} & & 1\cdots1 & & 0\\
& & & & 1\cdots1 & 0
\end{bmatrix}
\begin{matrix} \leftarrow 1 \\ \vdots \\ \vdots \\ \leftarrow r+1 \\ \vdots \\ \vdots \\ \vdots \\ \leftarrow n \end{matrix}$$

with all zero rows preceding all nonzero rows, where $r \geqslant 2$ *is the number of leaves in the tree T.*

Note that in general it is possible to have more than one permutation P such that (1) holds for all $x \in \mathbb{R}^n_{+\uparrow}$. Nevertheless, by Theorem 2.1, the adjacency matrices giving the maximum in (1) are always in the form satisfying conditions (I) and (II), and thus are all equal.

We first prove the necessity part of Theorem 2.1. The proof depends on the following lemma, where $A(1)$ denotes the submatrix of A with row and column 1 deleted.

Lemma 2.2. *Given any real* $n \times n$ *matrix A, suppose that for all* $x \in \mathbb{R}^n_{+\uparrow}$

$$x^{\mathrm{t}}Ax = \max\left\{x^{\mathrm{t}}Q^{\mathrm{t}}AQx\colon\ Q \in S_n\right\}.$$

Then for all $y \in \mathbb{R}^{n-1}_{+\uparrow}$

$$y^{\mathrm{t}}A(1)y = \max\left\{y^{\mathrm{t}}R^{\mathrm{t}}A(1)Ry\colon\ R \in S_{n-1}\right\}.$$

Proof. For any $y \in \mathbb{R}^{n-1}_{+\uparrow}$ it follows that

$$\begin{pmatrix} 0 \\ y \end{pmatrix} \in \mathbb{R}^n_{+\uparrow}.$$

Hence, for any $R \in S_{n-1}$

$$\begin{aligned} y^{\mathrm{t}} A(1) y &= \begin{pmatrix} 0 \\ y \end{pmatrix}^{\mathrm{t}} A \begin{pmatrix} 0 \\ y \end{pmatrix} \\ &\geqslant \begin{pmatrix} 0 \\ y \end{pmatrix}^{\mathrm{t}} \big([1] \oplus R^{\mathrm{t}}\big) A([1] \oplus R) \begin{pmatrix} 0 \\ y \end{pmatrix} \\ &= y^{\mathrm{t}} R^{\mathrm{t}} A(1) R y. \qquad \square \end{aligned}$$

Proof of the necessity part of Theorem 2.1. Assuming that for all $x \in \mathbb{R}^n_{+\uparrow}$

$$x^{\mathrm{t}} A x \geqslant x^{\mathrm{t}} Q^{\mathrm{t}} A Q x \quad \forall Q \in S_n,$$

we first prove condition (I), i.e., if $k_1 < k_2$ are two vertices of the tree T, then $\deg(k_1) \leqslant \deg(k_2)$. For $i = 1, 2$, define

$$u_i = \Big|\big\{u \neq k_1, k_2;\ u \leqslant k_1,\ u \text{ is adjacent to } k_i\big\}\Big|,$$

$$v_i = \Big|\big\{u \neq k_1, k_2;\ u > k_1,\ u \text{ is adjacent to } k_i\big\}\Big|.$$

Then for $i = 1, 2$

$$\deg(k_i) = \begin{cases} u_i + v_i, & (k_1, k_2) \text{ is not an edge,} \\ u_i + v_i + 1, & (k_1, k_2) \text{ is an edge.} \end{cases}$$

Consider

$$x = \Big(\overbrace{1, \ldots, 1}^{k_1}, 1 + \varepsilon, \ldots, 1 + \varepsilon\Big)^{\mathrm{t}},$$

where $\varepsilon > 0$. Let $Q \in S_n$ correspond to the transposition interchanging k_1 and k_2. Then

$$x^{\mathrm{t}} A x = 2\big(x_{k_1}(u_1 + (1+\varepsilon)v_1) + x_{k_2}(u_2 + (1+\varepsilon)v_2)\big) + \Delta$$

and

$$x^{\mathrm{t}} Q^{\mathrm{t}} A Q x = 2\big(x_{k_2}(u_1 + (1+\varepsilon)v_1) + x_{k_1}(u_2 + (1+\varepsilon)v_2)\big) + \Delta,$$

where Δ contains all terms not involving exactly one of x_{k_1} and x_{k_2}. Hence,

$$0 \leqslant x^{\mathrm{t}} A x - x^{\mathrm{t}} Q^{\mathrm{t}} A Q x = 2(x_{k_2} - x_{k_1})\big((u_2 - u_1) + (1+\varepsilon)(v_2 - v_1)\big),$$

which implies

$$(u_2 - u_1) + (1+\varepsilon)(v_2 - v_1) \geqslant 0.$$

Letting $\varepsilon \to 0$ gives $\deg(k_2) - \deg(k_1) \geqslant 0$, thus condition (I) holds and (since every tree has at least two leaves) vertices one and two of T are leaves.

Next we prove condition (II) by induction on n. The statement is clear if $n = 3$. Assume that the statement is true for $n - 1$, and let A be $n \times n$, where $n \geqslant 4$. As vertex 1 is a leaf, it follows that $A(1)$ is the adjacency matrix of the tree $T\backslash\{1\}$. By Lemma 2.2, we can apply the induction assumption on $A(1)$ to conclude that $A(1)$ satisfies condition (II), and hence $A(1) = L_1 + L_1^{\mathrm{t}}$, where

$$L_1 = \begin{bmatrix} 0\cdots0 & 0\cdots0 & \cdots & 0\cdots0 & 0\cdots0 & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0\cdots0 & 0\cdots0 & \cdots & 0\cdots0 & 0\cdots0 & 0\\ 1\cdots1 & & & & & 0\\ & 1\cdots1 & & & \text{\Large 0} & 0 \\ & & \ddots & & & \vdots \\ & \text{\Large 0} & & 1\cdots1 & & 0 \\ & & & & 1\cdots1 & 0 \end{bmatrix} \begin{matrix} \leftarrow 2 \\ \vdots \\ \vdots \\ \leftarrow r_2 \\ \vdots\\ \vdots \\ \vdots \\ \leftarrow n\end{matrix}$$

with $(r_2, 2)$ being the position of the unique nonzero entry in the first column. Note that the rows and columns of $A(1)$ are indexed by $2, 3, \ldots, n$.

Now

$$A = \begin{bmatrix} 0 & 0\cdots0\;1\;0\cdots0 \\ 0 & \\ \vdots & \\ 0 & \\ 1 & A(1) \\ 0 & \\ \vdots & \\ 0 & \end{bmatrix} = \begin{bmatrix} 0 & 0\cdots0\;1\;0\cdots0 \\ 0 & \\ \vdots & \\ 0 & \\ 1 & L_1 + L_1^{\mathrm{t}} \\ 0 & \\ \vdots & \\ 0 & \end{bmatrix}.$$

Hence, A can be written as $L + L^{\mathrm{t}}$, where

$$L = \begin{bmatrix} 0 & 0\cdots\;0\;\cdots0 \\ 0 & \\ \vdots & \\ 0 & \\ 1 & L_1 \\ 0 & \\ \vdots & \\ 0 & \end{bmatrix}$$

with $(r_1, 1)$ being the position of the unique nonzero entry in the first column. We claim that $r_1 = r_2$ or $r_2 - 1$ and consequently A satisfies condition (II). First, let $Q \in S_n$ correspond to the transposition that interchanges r_1 and r_2. Then

$$x^{\mathrm{t}}Ax = 2(x_1x_{r_1} + x_2x_{r_2}) + \varDelta$$

and

$$x^{\mathrm{t}}Q^{\mathrm{t}}AQx = 2(x_1x_{r_2} + x_2x_{r_1}) + \varDelta,$$

where $\varDelta$ contains all terms not involving exactly one of x_1 and x_2.

Hence, letting $x = (1, \ldots, n)^{\mathrm{t}}$,

$$0 \leqslant x^{\mathrm{t}}Ax - x^{\mathrm{t}}Q^{\mathrm{t}}AQx = 2(x_{r_2} - x_{r_1})(x_2 - x_1) = 2(r_2 - r_1)(2 - 1),$$

and thus $r_1 \leqslant r_2$. If $r_1 \leqslant r_2 - 2$, note that from L_1 we have $\deg_{T\setminus\{1\}}(s) = 1$ for $2 \leqslant s \leqslant r_2 - 1$. Therefore,

$$\deg_T(r_1) = \deg_{T\setminus\{1\}}(r_1) + 1 = 2 > 1 = \deg_{T\setminus\{1\}}(r_2 - 1) = \deg_T(r_2 - 1),$$

which contradicts condition (I). As a result, $r_1 = r_2$ or $r_2 - 1$. □

The proof of the sufficiency part of Theorem 2.1 is more intricate. In particular, we need to replace conditions (I) and (II) by some other conditions that are more convenient to use. First of all, it is not difficult to verify that conditions (I) and (II) are equivalent to condition (I) and th following condition (II′).

(II′) *If* (r_1, s_1) *and* (r_2, s_2) *are two positions of nonzero entries in A such that* $r_1 > s_1$ *and* $r_2 > s_2$, *then* $r_2 > r_1$ *implies that* $s_2 > s_1$.

We are going to describe another set of conditions equivalent to conditions (I) and (II), and the description requires the following definition.

Let $[k_1, k_2, \ldots, k_s]$ denote a path in a tree *T* connecting the vertices $k_1, k_2, \ldots, k_s$. A *maximal* path in *T* is a path that cannot be extended to a longer path. A path in *T* is thus maximal if and only if the two end vertices are leaves in *T*. It will be shown in Lemma 2.4 that conditions (I) and (II) are equivalent to condition (I) and the following condition (II″) in terms of the maximal paths in the tree *T* (cf. Theorem 1.3).

(II″) *If* $[k_1, k_2, \ldots, k_s]$ *is a maximal path in T labelled according to the row indices of the adjacency matrix A, then either*

$$k_1 < k_s < k_2 < k_{s-1} < \cdots \quad \textit{or} \quad k_s < k_1 < k_{s-1} < k_2 < \cdots$$

Note that either of the chains of inequalities in (II″) holds if and only if the submatrix of *A* lying in rows and columns with indices $k_1, k_s, k_2, k_{s-1}, \ldots$ or $k_s, k_1, k_{s-1}, k_2, \ldots$, respectively, is in the form displayed in Theorem 1.4.

The following technical lemma is needed to prove that conditions (I) and (II) are equivalent to conditions (I) and (II″).

Lemma 2.3. *Let A be the adjacency matrix of a tree T with vertices* $\{1, \ldots, n\}$ *labelled according to the row indices of A. If A satisfies condition* (II), *then the following are true*:

(a) *If* $[k_1, \ldots, k_s]$ *is a subpath of T, then for any* $1 < r < s$, *either* $k_1 < k_2 < \cdots < k_r$ *or* $k_r > k_{r+1} > \cdots > k_s$ *and, in particular, either* $k_1 < k_r$ *or* $k_r > k_s$.

(b) *If* $i < j$ *are vertices in T and k, l are adjacent to i, j, respectively, such that k and l do not lie on the unique path in T connecting i and j, then* $k < l$.

Proof. Note that if $[k_1, k_2, k_3]$ is a subpath of T, then the (k_1, k_2) and (k_3, k_2) entries of A are 1. Since no column of A has two 1's below the diagonal, then either $k_1 < k_2$ or $k_3 < k_2$. Now suppose $[k_1, \ldots, k_s]$ is a subpath of T and $1 < r < s$. Applying the previous argument to $[k_{r-1}, k_r, k_{r+1}]$ gives $k_{r-1} < k_r$ or $k_{r+1} < k_r$. If $k_{r-1} < k_r$, then consider $[k_{r-2}, k_{r-1}, k_r]$, $[k_{r-3}, k_{r-2}, k_{r-1}], \ldots, [k_1, k_2, k_3]$ giving $k_1 < k_2 < \cdots < k_r$; if $k_{r+1} < k_r$, then consider $[k_r, k_{r+1}, k_{r+2}]$, $[k_{r+1}, k_{r+2}, k_{r+3}], \ldots, [k_{s-2}, k_{s-1}, k_s]$ giving $k_r > k_{r+1} > \cdots > k_s$. Hence, condition (a) is proved.

Given i, j, k, l as in condition (b), applying condition (a) to the subpath $[k, i, \ldots, j, l]$ with $k_r = j$ gives $k < i < j$. If $l > j$, then condition (b) is proved, so suppose $l < j$. Then (i, k) and (j, l) are two nonzero entries of A below the diagonal with $i < j$, hence $k < l$, and condition (b) is proved. □

Lemma 2.4. *Let A be the adjacency matrix of a tree T with vertices* $\{1, \ldots, n\}$ *labelled according to the row indices of A. Then conditions* (I) *and* (II) *are equivalent to conditions* (I) *and* (II$''$).

Proof. Suppose condition (I) holds.

(II) $\Rightarrow$ (II$''$): Consider a maximal path $[k_1, \ldots, k_s]$ in T. If $k_1 < k_s$, then relabel the path as $[v_1, v_3, \ldots, v_4, v_2]$; if $k_1 > k_s$, then relabel the path as $[v_2, v_4, \ldots, v_3, v_1]$. We claim that $v_1 < v_2 < \cdots < v_s$ and thus (II$''$) follows. By construction, $v_1 < v_2$. As v_2 is a leaf but v_3 is not, $v_2 < v_3$ because the row sums of A are nondecreasing. Let k be the largest integer such that $v_1 < v_2 < \cdots < v_k$. If $k = s$, then the claim is proved. Otherwise, assume $k < s$. Note that $[v_{k-1}, v_{k+1}, \ldots, v_k]$ is a subpath and hence either $v_{k+1} > v_k$ or $v_{k+1} > v_{k-1}$ by Lemma 2.3(a). In the latter case, (v_{k+1}, v_{k-1}) and (v_k, v_{k-2}) are nonzero entries in the strictly lower triangular part of A and $v_{k-1} > v_{k-2}$, so we have $v_{k+1} \geqslant v_k$ by condition (II). Hence, $v_1 < \cdots < v_k < v_{k+1}$, contradicting the definition of k. Thus, our claim is proved.

(II$''$) $\Rightarrow$ (II): Suppose that (r_1, s_1) and (r_2, s_2) are positions of nonzero entries of A with $r_2 > r_1 > s_1$ and $r_2 > s_2$. Considering a maximal path γ containing (r_1, s_1) and (r_2, s_2), and the submatrix of A corresponding to γ as in condition (II$''$), gives $s_2 > s_1$. Thus, condition (II$'$) is true. Since conditions (I) and (II) are equivalent to conditions (I) and (II$'$) as already stated, the result follows. □

To utilize condition (II$''$) in the proof of the sufficiency part of Theorem 2.1, we need to understand the relation between a quadratic form $x^{\mathrm{t}}Ax$ and a given *maximal* path γ in T. This motivates the following partition of the matrix A according to γ and some lemmas associated with it. Let k be a vertex in T, and let $d(k, \gamma)$ be the length of the path joining k to a vertex in γ. Set $\mathscr{P}_j = \{k\colon\ d(k, \gamma) = j\}$ for $j = 0, \ldots, m$, where $m = \max_{1 \leqslant k \leqslant n}\ d(k, \gamma)$. Then $\{\mathscr{P}_0, \ldots, \mathscr{P}_m\}$ forms a partition of the vertex set $\{1, \ldots, n\}$. Let $A[\mathscr{P}_j; \mathscr{P}_k]$ be the submatrix of A lying in rows and columns indexed by elements in $\mathscr{P}_j$ and $\mathscr{P}_k$, respectively.

For example, the adjacency matrix A given by

$$\begin{bmatrix} 0 & 1 & 1 & | & 1 & 1 & | & 0 \\ 1 & 0 & 0 & | & 0 & 0 & | & 0 \\ 1 & 0 & 0 & | & 0 & 0 & | & 0 \\ - & - & - & - & - & - & - & - \\ 1 & 0 & 0 & | & 0 & 0 & | & 0 \\ 1 & 0 & 0 & | & 0 & 0 & | & 1 \\ - & - & - & - & - & - & - & - \\ 0 & 0 & 0 & | & 0 & 1 & | & 0 \end{bmatrix}$$

illustrates the partition $\mathscr{P}_0 = \{1, 2, 3\}$, $\mathscr{P}_1 = \{4, 5\}$ and $\mathscr{P}_2 = \{6\}$ with respect to $\gamma = [2, 1, 3]$, and the properties (a)–(f) in the following lemma.

Lemma 2.5. *For the partition $\mathscr{P}_0, \ldots, \mathscr{P}_m$ defined above, the following are true*:

(a) *If $j \geqslant 1$, then $A[\mathscr{P}_j; \mathscr{P}_j] = 0$.*

(b) *If $|j - k| > 1$, then $A[\mathscr{P}_j; \mathscr{P}_k] = 0$.*

(c) *For $j = 0, \ldots, m - 1$, every column in $A[\mathscr{P}_j; \mathscr{P}_{j+1}]$ has exactly one* 1.

(d) *For $j = 1, \ldots, m - 1$, each row sum of $A[\mathscr{P}_j; \mathscr{P}_{j+1}]$ is one less than the corresponding row sum of A.*

(e) *The two rows in $A[\mathscr{P}_0; \mathscr{P}_1]$ corresponding to the two leaves in γ are* 0. *Every other row sum of $A[\mathscr{P}_0; \mathscr{P}_1]$ is two less than the corresponding row sum of A.*

(f) *If A has nondecreasing row sums, then so does $A[\mathscr{P}_j; \mathscr{P}_{j+1}]$ for $j = 0, \ldots, m - 1$.*

Proof. (a) For $j \geqslant 1$, no two vertices in $\mathscr{P}_j$ are adjacent, otherwise there is a cycle in T.

(b) If there exists a vertex $v \in \mathscr{P}_k$ adjacent to a vertex $w \in \mathscr{P}_j$, then by the construction of the partition, either $v \in \mathscr{P}_{j+1}$ or $v \in \mathscr{P}_{j-1}$.

(c) No two vertices in $\mathscr{P}_j$ can be adjacent to the same vertex in $\mathscr{P}_{j+1}$, otherwise a cycle exists in T; and each vertex in $\mathscr{P}_{j+1}$ is adjacent to one vertex in $\mathscr{P}_j$.

(d) For $1 \leqslant j \leqslant m - 1$, each vertex k in $\mathscr{P}_j$ is adjacent to $\deg(k) - 1$ vertices in $\mathscr{P}_{j+1}$. Note that each vertex is adjacent to one vertex in $\mathscr{P}_{j-1}$.

(e) Each vertex k in $\mathscr{P}_0$, except the two leaves, is adjacent to $\deg(k) - 2$ vertices in $\mathscr{P}_1$. Note that each vertex, except the two leaves, is adjacent to two other vertices in $\mathscr{P}_0$.

(f) Suppose r and s are in $\mathscr{P}_j$. If the row sum of A corresponding to r is greater than or equal to that corresponding to s, then by property (d) if $j \neq 0$ or by property (e) if $j = 0$, the row sum in $A[\mathscr{P}_j; \mathscr{P}_{j+1}]$ corresponding to r is greater than or equal to that corresponding to s. □

Lemma 2.6. *Given positive integers* $p \leqslant q$ *and* $0 \leqslant m_1 \leqslant \cdots \leqslant m_p$ *such that* $m_1 + \cdots + m_p = q$, *consider the* $p \times q$ *matrix*

$$B = \begin{bmatrix} \overbrace{1\cdots 1}^{m_1} & \overbrace{0\cdots 0}^{m_2} & \cdots & \overbrace{0\cdots 0}^{m_{p-1}} & \overbrace{0\cdots 0}^{m_p} \\ & 1\cdots 1 & & & \\ & & \ddots & \text{0} & \\ & \text{0} & & 1\cdots 1 & \\ & & & & 1\cdots 1 \end{bmatrix}.$$

Then for any $x \in \mathbb{R}^p_{+\uparrow}$ *and* $y \in \mathbb{R}^q_{+\uparrow}$

$$x^{\mathrm{t}} B y \geqslant x^{\mathrm{t}} P^{\mathrm{t}} B Q y \quad \forall P \in S_p \ \text{ and } \ \forall Q \in S_q.$$

Proof. Write $Px = (f_1, \dots, f_p)^{\mathrm{t}}$ and $Qy = (g_1^{\mathrm{t}}, \dots, g_p^{\mathrm{t}})^{\mathrm{t}}$, where g_i is a vector of length m_i for $i = 1, \dots, p$. Let $1 \leqslant i < j \leqslant p$. Then

$$x^{\mathrm{t}} P^{\mathrm{t}} B Q y = f_1 \Big(\overbrace{11\cdots 1}^{m_1}\Big) g_1 + \cdots + f_i \Big(\overbrace{11\cdots 1}^{m_i}\Big) g_i + \cdots + f_j \Big(\overbrace{11\cdots 1}^{m_j}\Big) g_j + \cdots + f_p \Big(\overbrace{11\cdots 1}^{m_p}\Big) g_p$$

is maximal only if for all $i < j$, $f_i \leqslant f_j$ and the sum of the entries of g_i is not larger than the sum of the entries of g_j. The latter is true if $y \in \mathbb{R}^q_{+\uparrow}$, hence the result follows. □

We are now ready to present:

Proof of the sufficiency part of Theorem 2.1. Suppose A satisfies conditions (I) and (II), or equivalently by Lemma 2.4, conditions (I) and (II$''$). Let $x \in \mathbb{R}^n_{+\uparrow}$. Consider the set

$$\mathbb{S}(x) = \left\{ \hat{P} \in S_n\colon\ x^{\mathrm{t}} \hat{P}^{\mathrm{t}} A \hat{P} x \geqslant x^{\mathrm{t}} Q^{\mathrm{t}} A Q x \ \forall Q \in S_n \right\}.$$

If $I \in \mathbb{S}(x)$ for every $x \in \mathbb{R}^n_{+\uparrow}$, then the result holds. So suppose that there exists $x \in \mathbb{R}^n_{+\uparrow}$ such that $I \notin \mathbb{S}(x)$. For notational simplicity, we let $\mathbb{S} = \mathbb{S}(x)$. Define, for each $\hat{P} \in \mathbb{S}$,

$$b(\hat{P}) = \min \left\{ t\colon\ \hat{P} e_t \neq e_t \right\},$$

where $e_1, \dots, e_n$ are the standard orthonormal basis vectors of $\mathbb{R}^n$. Let $\tilde{P} \in \mathbb{S}$ satisfy $b(\tilde{P}) \geqslant b(\hat{P})$ for all $\hat{P} \in \mathbb{S}$. We will show that there exists $R \in \mathbb{S}$ with $b = b(\tilde{P}) < b(R)$, which gives the desired contradiction, and thus $I \in \mathbb{S}$ for all $x \in \mathbb{R}^n_{+\uparrow}$.

Choose a maximal path γ in T containing b and c, where $\tilde{P} e_b = e_c$. Note that $b < c$. With γ, construct the partition $\mathscr{P}_0, \dots, \mathscr{P}_m$ as above Lemma 2.5. If (v_1, w_1)

and (v_2, w_2) are two nonzero entries of $A[\mathscr{P}_j; \mathscr{P}_{j+1}]$ with $v_1 < v_2$, then by the construction of the partition and the fact that A satisfies condition (II), Lemma 2.3(b) implies that $w_1 < w_2$. Using Lemma 2.5(c), it follows that $A[\mathscr{P}_j; \mathscr{P}_{j+1}]$ is in row echelon form. By condition (I) and Lemma 2.5(f), $A[\mathscr{P}_j; \mathscr{P}_{j+1}]$ is in row echelon form with nondecreasing row sums.

Given $y \in \mathbb{R}^n$, let $y_{\mathscr{P}_j}$ be the vector obtained from y by retaining in order the entries corresponding to the indices in $\mathscr{P}_j$. We define a vector z as follows. For $j = 0, \ldots, m$, let Q_j be a permutation matrix such that

$$Q_j\big(\tilde{P}x\big)_{\mathscr{P}_j} = z_{\mathscr{P}_j}$$

is in nondecreasing order. Let $R \in S_n$ be such that $Rx = z = (z_1, \ldots, z_n)^{\mathrm{t}}$.

To prove $R \in \mathbb{S}$, i.e., $x^{\mathrm{t}}R^{\mathrm{t}}ARx = x^{\mathrm{t}}\tilde{P}^{\mathrm{t}}A\tilde{P}x$, note that by Lemma 2.5(a) and (b),

$$x^{\mathrm{t}}R^{\mathrm{t}}ARx = z^{\mathrm{t}}Az = z^{\mathrm{t}}_{\mathscr{P}_0}A[\mathscr{P}_0; \mathscr{P}_0]z_{\mathscr{P}_0} + 2\sum_{j=0}^{m-1} z^{\mathrm{t}}_{\mathscr{P}_j}A[\mathscr{P}_j; \mathscr{P}_{j+1}]z_{\mathscr{P}_{j+1}}.$$

Since γ is a maximal path, by (II$''$) and Theorem 1.4,

$$z^{\mathrm{t}}_{\mathscr{P}_0}A[\mathscr{P}_0; \mathscr{P}_0]z_{\mathscr{P}_0} \geqslant \big(\tilde{P}x\big)^{\mathrm{t}}_{\mathscr{P}_0}A[\mathscr{P}_0; \mathscr{P}_0]\big(\tilde{P}x\big)_{\mathscr{P}_0}.$$

Also since $A[\mathscr{P}_j; \mathscr{P}_{j+1}]$ is in row echelon form with nondecreasing row sums, by Lemma 2.6,

$$z^{\mathrm{t}}_{\mathscr{P}_j}A[\mathscr{P}_j; \mathscr{P}_{j+1}]z_{\mathscr{P}_{j+1}} \geqslant \big(\tilde{P}x\big)^{\mathrm{t}}_{\mathscr{P}_j}A[\mathscr{P}_j; \mathscr{P}_{j+1}]\big(\tilde{P}x\big)_{\mathscr{P}_{j+1}}.$$

It follows that

$$\begin{aligned} x^{\mathrm{t}}R^{\mathrm{t}}ARx &\geqslant \big(\tilde{P}x\big)^{\mathrm{t}}_{\mathscr{P}_0}A[\mathscr{P}_0; \mathscr{P}_0]\big(\tilde{P}x\big)_{\mathscr{P}_0} \\ &\quad + 2\sum_{j=0}^{m-1}\big(\tilde{P}x\big)^{\mathrm{t}}_{\mathscr{P}_j}A[\mathscr{P}_j; \mathscr{P}_{j+1}]\big(\tilde{P}x\big)_{\mathscr{P}_{j+1}} \\ &= x^{\mathrm{t}}\tilde{P}^{\mathrm{t}}A\tilde{P}x. \end{aligned}$$

Since $\tilde{P} \in \mathbb{S}$, we have $x^{\mathrm{t}}R^{\mathrm{t}}ARx = x^{\mathrm{t}}\tilde{P}^{\mathrm{t}}A\tilde{P}x$.

To prove $b(R) > b = b(\tilde{P})$, write $\tilde{P}x = (y_1, \ldots, y_n)^{\mathrm{t}}$. By the definition of b,

$$\begin{array}{ccccccccccc} y_1 & \leqslant & y_2 & \leqslant & \cdots & \leqslant & y_{b-1} & \leqslant & y_c & \leqslant & y_j \quad \text{whenever } j \geqslant b \\ \| & & \| & & & & \| & & \| & & \\ x_1 & \leqslant & x_2 & \leqslant & \cdots & \leqslant & x_{b-1} & \leqslant & x_b & & \end{array}.$$

Suppose $s < b$, $s \in \mathscr{P}_j$ for some $0 \leqslant j \leqslant m$, and $\mathscr{P}_j$ has indices $s_1 < \cdots < s_u$ with $s_u = s$. Then for $s_k > s_u = s$

$$y_{s_1} \leqslant \cdots \leqslant y_{s_u} \leqslant y_{s_k}.$$

So the choice of $z_{\mathscr{P}_j}$ implies $z_{s_l} = y_{s_l} = x_{s_l}$ for $s_l \leqslant s_u = s < b$. It follows that we may take $Re_s = e_s$ for $s < b$. If $s = b$, then since b and c are in $\mathscr{P}_0$, a similar argument gives

$$y_{s_1} \leqslant \cdots \leqslant y_{s_{u-1}} \leqslant y_c \leqslant y_{s_k}$$

for $s_k \geqslant s_u = b$. Our choice of $z_{\mathscr{P}_0}$ implies that $z_b = z_{s_u} = y_c = x_b$. It follows that we may take $Re_b = e_b$ and thus $b(R) > b$ contradicting the maximality of $b(\tilde{P})$. □

3. Optimal labelling of trees

An adjacency matrix A of a tree T is said to be an *optimal* adjacency matrix if it satisfies conditions (I) and (II). If A is an optimal adjacency matrix, then the tree T labelled according to the row indices of A is said to have an *optimal labelling*. The following result characterizes those trees T that have an optimal labelling.

Theorem 3.1. *A tree T has an optimal labelling if and only if it is isomorphic to a rooted tree depicted with the root at the top level and leaves at the bottom level such that there are no crossing edges and the following properties are satisfied*:

(P1) *In each level, the degrees of vertices are nonincreasing from left to right.*

(P2) *Each vertex in a higher level has degree greater than or equal to that of each vertex in a lower level.*

Proof. (⇒): Suppose T has vertex set $\{1, \ldots, n\}$ labelled according to the row indices of an optimal adjacency matrix A. Let vertex n, a vertex with maximal degree, be the root vertex and put it in the top level. Once a certain level of vertices has been determined, arrange the vertices in the next level as follows. For each vertex in the current level starting from the left end, collect the vertices that are adjacent to it and arrange them in the next level so that their indices are nonincreasing from left to right. We claim that the resulting tree satisfies properties (P1) and (P2). To this end, we first prove the following result.

(P3) *Any vertex $v < n$ is either on the right of $v + 1$ or in a level lower than $v + 1$.*

It is true for $v = n - 1$. Suppose it is true for any vertex $u \geqslant v + 1$. By condition (II) if $v + 1$ is adjacent to $r > v + 1$, then either (i) v is adjacent to r or (ii) v is adjacent to $r - 1$. If (i) holds or (ii) holds with $r - 1$ on the right of r, then v is on the right of $v + 1$ by our construction. If (ii) holds and $r - 1$ is in a level lower than r, then v is in a level lower than $v + 1$. Thus (P3) holds.

Now for any vertices u_1 and u_2 with $\deg(u_1) > \deg(u_2)$, by condition (I) $u_1 > u_2$ and, by considering $u_2, u_2 + 1, \ldots, u_1 - 1, u_1$ and (P3), u_2 is on the right or is in a level lower than u_1. Thus, (P1) and (P2) are true, and the claim is proved.

(⇐): Given a rooted tree with n vertices and (P1) and (P2), label the root vertex as n. Label the n_1 vertices in the second level, the n_2 vertices in the third level, and so on, from left to right, by $\{n - 1, \ldots, n - n_1\}$, $\{n - n_1 - 1, \ldots, n - n_2\}$, and so on. Let A be the corresponding adjacency matrix. The row sums of A are nondecreasing by (P1) and (P2). To prove condition (II), suppose (r_1, s_1) and (r_2, s_2) are nonzero entries in A such that $r_1 > s_1$ and $r_2 > s_2$. Assume that $r_2 > r_1$. In the labelled tree, either vertex r_2 is to the left of vertex r_1 (in the same level), and thus $s_2 > s_1$ as there are no crossing edges; or vertex r_2 is in a level above vertex r_1, and again $s_2 > s_1$. □

Note that (P1) and (P2) together imply that the root is a vertex with maximal degree, and only the vertices in the lowest (bottom) two levels can be leaves. Moreover, an optimal labelling is a monotone ordering and a minimum degree ordering (see [4]). Let $\deg(v)$ denote the degree of vertex v in T. The following corollary follows from properties (I) and (II$''$) of an optimal adjacency matrix.

Corollary 3.2. *Suppose T has an optimal labelling. Then the following are true*:

(a) *In any path in T, there cannot be a vertex with lower degree lying between two vertices with higher degree.*

(b) *For every maximal path* $[k_1, k_2, \ldots, k_s]$ *in T,*

$$1 = \deg(k_1) = \deg(k_s) \leqslant \deg(k_2) \leqslant \deg(k_{s-1}) \leqslant \cdots$$

or

$$1 = \deg(k_s) = \deg(k_1) \leqslant \deg(k_{s-1}) \leqslant \deg(k_2) \leqslant \cdots.$$

(c) *If there exists a unique vertex v with maximal degree, then it is a center of every maximal path passing through it.*

We now use Theorem 3.1 to give optimal labellings for some families of trees.

Example 3.3. Let T be a path with n vertices. An optimal labelling is given by taking a center vertex as the root with label n; its neighbors in the next level with labels $n-1, n-2$; their other neighbors in the next level with labels $n-3, n-4$, respectively; and so on. If n is odd, then both leaves are in the same bottom level; if n is even, then the lowest leaf with label 1 is one level lower than the leaf with label 2.

Example 3.4. Let T be a star with n vertices. Then an optimal labelling is given by taking the center vertex as the root with label n, and giving labels $1, \ldots, n-1$ to its neighbors (leaves) in any order.

Example 3.5. Let $T(n; p, q, r)$ denote a tree with $n \geqslant 5$ vertices obtained from a star on $q+r+1$ vertices by inserting $p \geqslant 1$ additional vertices on each of $q \geqslant 1$ edges and $p-1$ additional vertices on each of the remaining $r \geqslant 0$ edges. Thus, $n = rp + 1 + q(1+p)$, and T has q leaves in the bottom level with r leaves in one level higher. Then an optimal labelling for $T(n; p, q, r)$ is given by taking the center vertex of the star as the root with label n, giving labels $n-1, \ldots, n-q$ to its neighbors on the edges with p vertices inserted, labels $n-q-1, \ldots, n-q-r$ to

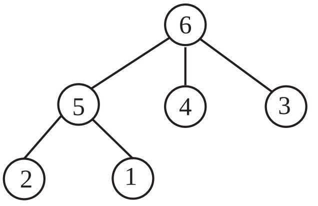

Fig. 1.

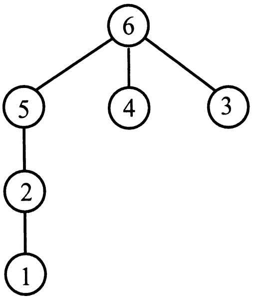

Fig. 2.

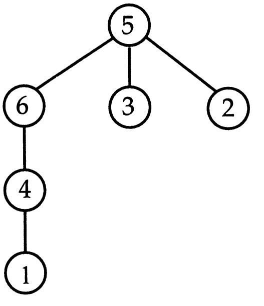

Fig. 3.

its neighbors on the edges with $p-1$ vertices inserted, and continuing to label their neighbors in the same order. If $r \geqslant 1$, the leaves are in the two lowest levels.

Examples 3.3–3.5 can be used to give an optimal labelling for all trees with at most five vertices, and for four of the six trees with six vertices. For a list of trees with at most 10 vertices see [2, Appendix, Table 2]. The only tree with three vertices is a path; there are two trees with four vertices, a path and a star; there are three trees with five vertices, a path, a star and $T(5; 1, 1, 2)$. Five of the six trees with six vertices have an optimal labelling: a path, a star, $T(6; 1, 1, 4)$, $T(6; 1, 2, 1)$, and the tree (not covered by the examples) given in Fig. 1.

Thus by Theorem 2.1, Problem 1.1 (and hence Problem 1.2) has a solution, and all labellings are characterized for each of the above trees so that the adjacency matrices satisfy conditions (I) and (II). The one tree with six vertices that does not have an optimal labelling is listed as 2.11 in [2, Appendix, Table 2]; we will return to this in Section 4 (see Figs. 2 and 3). Seven of the 11 trees with seven vertices (five of which are covered by the above examples) have an optimal labelling, and hence have a solution to Problems 1.1 and 1.2. The remaining four trees with seven vertices that have no optimal labelling are listed as 2.17, 2.19, 2.21 and 2.22 in [2, Appendix, Table 2].

4. Related results

Even if Problem 1.1 does not have a solution, but we know that $\max\{x^{\mathrm{t}}Q^{\mathrm{t}}AQx\colon\ Q \in S_n\}$ can only occur for $Q \in \{P_1, \ldots, P_k\}$, then we have a corresponding result for Problem 1.2. Here k is usually small compared with $n!$. The proof of the following proposition parallels that of Proposition 1.5.

Proposition 4.1. *Let A be an adjacency matrix of a tree T with n vertices. Suppose permutation matrices* $P_1, \ldots, P_k \in S_n$ *are such that for all* $x \in \mathbb{R}^n_{+\uparrow}$

$$\max_{1\leqslant j\leqslant k} x^{\mathrm{t}}P_j^{\mathrm{t}}AP_jx \geqslant x^{\mathrm{t}}Q^{\mathrm{t}}AQ \quad \forall Q \in S_n.$$

Then for all $D = \mathrm{diag}\,(d_1, \ldots, d_n)$ *with* $d_1 \leqslant \cdots \leqslant d_n$

$$\max_{1\leqslant j\leqslant k} \lambda_{\max}\big(D + P_j^{\mathrm{t}}AP_j\big) \geqslant \max_{1\leqslant j\leqslant k} \lambda_{\max}\big(D + Q^{\mathrm{t}}AQ\big) \quad \forall Q \in S_n.$$

As discussed at the end of Section 3, there is one tree with six vertices that does not have an optimal labelling (see [2, Appendix, Table 2, 2.11]). Problem 1.2 (and hence Problem 1.1) has no solution for this tree. Using Proposition 4.1, we can, however, narrow our search to two permutations P_1, P_2 to give $\max_{1\leqslant j\leqslant 2} \lambda_{\max}(D + P_j^{\mathrm{t}}AP_j)$. In fact, if $D = \mathrm{diag}\,(0, 0, 0, 0, 0, 1)$, then $\max \lambda_{\max}(D + P^{\mathrm{t}}AP)$ occurs for A labelled according to the tree in Fig. 2. If $D = \mathrm{diag}\,(0, 0, 0, 1, 1, 1,)$, then $\max \lambda_{\max}(D + P^{\mathrm{t}}AP)$ occurs for A labelled according to Fig. 3. Note that these are not optimal labellings since property (P2) is not satisfied.

Problems corresponding to 1.1 and 1.2 can also be considered for symmetric nonnegative matrices or for adjacency matrices of general graphs. For example, we give the solution to Problem 1.1 (and thus to Problem 1.2) for a class of matrices associated with the star graph (cf. [3, Theorem 4]), and for graphs on four vertices that contain a cycle.

Theorem 4.2. *Let*

$$B = \begin{pmatrix} 0_{n-1} & u \\ u^{\mathrm{t}} & 0 \end{pmatrix},$$

where $u = (u_1, \ldots, u_{n-1})^{\mathrm{t}}$ *with* $0 \leqslant u_1 \leqslant \cdots \leqslant u_{n-1}$. *Then for all* $x \in \mathbb{R}^n_{+\uparrow}$

$$x^{\mathrm{t}}Bx \geqslant x^{\mathrm{t}}Q^{\mathrm{t}}BQx \quad \forall Q \in S_n.$$

Consequently, for all $D = \mathrm{diag}(d_1, \ldots, d_n)$ *with* $d_1 \leqslant \cdots \leqslant d_n$

$$\lambda_{\max}(D + B) \geqslant \lambda_{\max}\big(QDQ^{\mathrm{t}} + B\big) \quad \forall Q \in S_n.$$

Proof. For any nonnegative $x = (x_1, \ldots, x_n)^{\mathrm{t}}$, $x^{\mathrm{t}}Q^{\mathrm{t}}BQx = 2(\sum_{j=1}^{n-1} u_jx_nx_j)$. This expression is maximized (among all permutations of the entries of x) when $x_1 \leqslant \cdots \leqslant x_n$. This gives the first assertion, and the second assertion follows easily from Proposition 1.5. □

Example 4.3. There are six graphs with four vertices: two trees; two graphs (the 4-cycle and the complete graph) for which all $P \in S_4$ solve Problems 1.1 and 1.2 due to symmetry; and two others (a 4-cycle with a chord and a kite graph, see 1.5 and 1.6, respectively, in [2, Appendix, Table 1]). For either of these latter two graphs, maximization of the quadratic form in Problem 1.1 gives an optimal labelling when the adjacency matrix has nondecreasing row sums. Thus, the problems corresponding to 1.1 and 1.2 have a solution for all graphs with four vertices.

We conclude by noting that the minimum of the smallest eigenvalue of matrices of the form $PDP^{\mathrm{t}} + A$ can be obtained from the following duality result. This dual problem for a path is the main focus of the work in [1,7].

Proposition 4.4. *Let A be an adjacency matrix of a tree with n vertices. If for all* $D = \mathrm{diag}(d_1, \ldots, d_n)$ *with* $d_1 \leqslant \cdots \leqslant d_n$

$$\lambda_{\max}\left(PDP^{\mathrm{t}} + A\right) \geqslant \lambda_{\max}\left(QDQ^{\mathrm{t}} + A\right) \quad \forall Q \in S_n,$$

then for all $D = \mathrm{diag}\,(d_1, \ldots, d_n)$ *with* $d_1 \geqslant \cdots \geqslant d_n$

$$\lambda_{\min}\left(PDP^{\mathrm{t}} + A\right) \leqslant \lambda_{\min}\left(QDQ^{\mathrm{t}} + A\right) \quad \forall Q \in S_n.$$

Proof. Since $PDP^{\mathrm{t}} + A$ is signature similar to $PDP^{\mathrm{t}} - A$, it follows that $\lambda_{\max}(PDP^{\mathrm{t}} + A) = -\lambda_{\min}(P(-D)P^{\mathrm{t}} + A)$, which gives the result. □

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