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# Matrices totally positive relative to a tree, II

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#### АВЅТ КАСТ

If T is a labelled tree, a matrix A is totally positive relative to T, principal submatrices of A associated with deletion of pendent vertices of T are P-matrices, and A has positive determinant, then the smallest absolute eigenvalue of A is positive with multiplicity 1 and its eigenvector is signed according to T. This conclusion has been incorrectly conjectured under weaker hypotheses.

Keywords: Graph Neumaier conclusion Spectral theory Sylvester's identity Totally positive matrix Totally positive relative to a tree

## 1. Introduction

A real matrix is called *totally positive* (TP) if all its minors are positive, and it is a P-matrix if every principal minor is positive.

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In [1] the following weakening has been studied. An *n*-by-*n* real matrix is *totally* positive relative to a given labelled tree T on n vertices (T-TP) if, for each pair of pendent vertices p and q of T, the matrix  $A[\alpha]$  is TP when  $\alpha$  is the ordered set of vertices of the unique induced path of T that connects p and q. If T is a path with vertices labelled in order, then TP and T-TP are the same. Note that we are going to refer to T throughout as a labelled tree.

Of course, T-TP equivalently means that  $A[\alpha]$  is TP for the vertices of any induced path of T, as the unique path joining any pair of vertices of T is a subpath of some path joining pendent vertices.

It is known that a totally positive matrix has distinct positive eigenvalues and that the smallest one has an eigenvector that alternates in sign (see [2] for general background). Since a tree is bipartite, there is a signing of the vertices so that neighbors have different signs. For a labelled tree, T, let  $\sigma$  be a  $\pm 1$  vector consistent with such a signing. We say that  $\sigma$  is signed according to T, and  $\sigma$  is unique up to multiplication by  $\pm 1$ . It had been conjectured that if A is T-TP, then A has a unique absolute smallest real eigenvalue with an eigenvector signed according to T. We call this the Neumaier conclusion, after the original conjecture by Arnold Neumaier, University of Vienna. See [1] for prior work.

This conjecture was proven for a few trees, but is false in general. Here, our purpose is to prove the original conjecture for all trees by adding a hypothesis.

### 2. Notation and terminology

Let us denote the set  $\{1, \ldots, n\}$  by N; Moreover, we will denote by  $N_i$  (resp.  $N_{i,j}$ , and  $N_{i,j,k}$ ) the set  $N \setminus \{i\}$  (resp.  $N \setminus \{i, j\}$ , and  $N \setminus \{i, j, k\}$ ).

Let  $A \in M_n(\mathbb{R})$ . For any ordered index sets  $\alpha, \beta \subseteq N$ , with  $|\alpha| = |\beta| = k$ , by  $A[\alpha; \beta]$ we mean the k-by-k submatrix of A that lies in the rows indexed by  $\alpha$  and the columns indexed by  $\beta$ , and with the order of the rows (resp. columns) determined by the order in  $\alpha$  (resp.  $\beta$ ), by  $A[\alpha]$  we mean  $A[\alpha; \alpha]$ , by A(i; j) we mean the (n-1)-by-(n-1) submatrix of A that lies in the rows indexed by  $N_i$  and the columns indexed by  $N_j$ , and by A(i)we mean A(i; i).

Suppose that T is a labelled tree on n vertices. If  $\mathscr{P}$  is an induced path of T, by  $A[\mathscr{P}]$  we mean  $A[\alpha]$  in which  $\alpha$  consists of the indices of the vertices of  $\mathscr{P}$  in the order in which they appear along  $\mathscr{P}$ . Since everything we discuss is independent of reversal of order, there is no ambiguity regarding intended direction.

**Definition 1.** For a given labelled tree T on n vertices, we say that  $A \in M_n(\mathbb{R})$  is T-TP if  $A[\mathscr{P}]$  is TP for each path  $\mathscr{P}$  connecting any two pendent vertices.

Observe that for a T-TP matrix, properly less is required than for a TP matrix; however, like TP matrices, T-TP matrices are entry-wise positive. **Definition 2.** For a given labelled tree T on n vertices, we say that  $A \in M_n(\mathbb{R})$  is pendent-P relative to T if all principal submatrices, associated with the deletion of pendent vertices, one at a time, are P-matrices.

Note that since in a P-matrix all the principal minors are positive the property of being pendent-P relative to a tree is preserved by permutation similarity.

**Definition 3.** For a given labelled tree T on n vertices, we say that  $A \in M_n(\mathbb{R})$  is T-positive if it is T-TP and pendent-P relative to T.

Our arguments strongly use the adjoint of a T-TP matrix (or one satisfying additional hypotheses) as a surrogate for the inverse, and we frequently use Sylvester's determinantal identity, along with ad hoc arguments, to determine the sign pattern of the adjoint.

The version of Sylvester's identity we shall use is the following [3, (0.8.6.1)]:

$$\det A[\alpha;\beta] = \frac{\det A[\alpha';\beta'] \det A[\alpha';\beta] - \det A[\alpha';\beta] \det A[\alpha;\beta']}{\det A[\alpha';\beta']},$$
(1)

in which  $\alpha$  and  $\beta$  are index sets of the same size,  $\alpha'$  (resp.  $\beta'$ ) is  $\alpha$  (resp.  $\beta$ ) without the last index; ' $\alpha$  (resp. ' $\beta$ ) is  $\alpha$  (resp.  $\beta$ ) without the first index, and ' $\alpha'$  (resp. ' $\beta'$ ) is  $\alpha$  (resp.  $\beta$ ) without the first index and last index. Note that, above, as throughout, these index sets are ordered. We also denote by  $\widetilde{A} = (\widetilde{a}_{i,j})$  the adjoint of A.

## 3. Main result

Our purpose here is to give hypotheses sufficient to achieve the Neumaier conclusion relative to any tree. Our approach is to give hypotheses so that  $SA^{-1}S$  is an entry-wise positive matrix where S is the signature matrix determined by  $\sigma$  signed according to T. By Perron's Theorem this means that the smallest eigenvalue is positive and has an eigenvector signed according to T. To this end our first result is.

**Theorem 4.** Let T be a labelled tree on n vertices and  $A \in M_n(\mathbb{R})$  be T-positive with det A > 0. Then

$$\operatorname{sign}(\det A(i;j)) = (-1)^{i+j} \sigma_i \sigma_j$$

in which  $\sigma$  is signed according to T.

**Remark 5.** It is important to point out the fact that  $(-1)^{i+j} \det A(j;i)$  is the (i,j) entry in the adjoint matrix of A, i.e.,

$$\det A(j;i) = (-1)^{i+j} \widetilde{a}_{i,j}.$$

For this reason we will write  $\tilde{a}_{i,j}$  instead of  $(-1)^{i+j} \det A(j;i)$  throughout the paper.

Now, let  $S_{\sigma} = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_n)$  with  $\sigma$  signed according to T. We have

**Corollary 6.** If T is a tree on n vertices and  $A \in M_n(\mathbb{R})$  is T-positive with det A > 0. Then

$$S_{\sigma}A^{-1}S_{\sigma}$$
 is entry-wise positive.

Therefore, A satisfies the Neumaier conclusion.

Notice that A is TP (P) matrix if and only if  $S_{\sigma}A^{-1}S_{\sigma}$  is so, see, e.g., [2, Theorem 1.3.3].

### 4. Supporting facts and proofs

In this section we give the results that we need in order to prove Theorem 4. We also deduce the corollaries from it. First we state a technical result we need to prove Lemma 9.

**Lemma 7.** Given a matrix  $A \in M_n(\mathbb{R})$ , then for any three distinct integers i, j, k, with  $1 \leq i, j, k \leq n$ , we have

$$\begin{aligned} \widetilde{a}_{k,i} \det A[i, N_{i,j,k}; i, N_{i,j,k}] \\ &+ \widetilde{a}_{k,j} \det A[j, N_{i,j,k}; i, N_{i,j,k}] + \widetilde{a}_{k,k} \det A[k, N_{i,j,k}; i, N_{i,j,k}] = 0. \end{aligned}$$

**Proof.** Without loss of generality we may assume that  $1 \le i < j < k \le n$ . To simplify the expressions we denote  $N_{i,j,k}$  by  $\alpha$ . By Sylvester's identity (1) and taking into account how the sign of the determinant changes after a permutation of the indices we get

$$\begin{split} \widetilde{a}_{k,j} &= (-1)^{k+j} (-1)^{2i-2} \det A[i, N_{i,j}; i, N_{i,k}] = (-1)^{n-1} \det A[i, N_{i,j,k}, k; j, i, N_{i,j,k}] \\ &= (-1)^n \frac{\det A[i, \alpha; i, \alpha] \det A[\alpha, k; j, i, \alpha'] - \det A[i, \alpha; j, i, \alpha'] \det A[\alpha, k; i, \alpha]}{\det A[\alpha; i, \alpha']} \\ &= \frac{\det A[i, \alpha; i, \alpha] \det A[\alpha, k; j, i, \alpha'] - \det A[i, \alpha; j, i, \alpha'] \det A[\alpha, k; i, \alpha]}{\det A[r, \alpha'; i, \alpha']}, \end{split}$$

where r is the last entry of  $\alpha$ .

On the other hand and following the same ideas as before, we get

$$\begin{split} \widetilde{a}_{k,i} &= (-1)^{k+i+1} \det A[j, N_{i,j}; j, N_{j,k}] = (-1)^n \det A[j, \alpha, k; j, i, \alpha] \\ &= (-1)^n \frac{\det A[j, \alpha; j, i, \alpha'] \det A[\alpha, k; i, \alpha] - \det A[j, \alpha; i, \alpha] \det A[\alpha, k; j, i, \alpha']}{\det A[\alpha; i, \alpha']} \\ &= \frac{\det A[j, \alpha; j, i, \alpha'] \det A[\alpha, k; i, \alpha] - \det A[j, \alpha; i, \alpha] \det A[\alpha, k; j, i, \alpha']}{\det A[r, \alpha'; i, \alpha']}. \end{split}$$

Thus using the last two expressions and combining them properly, we get

$$\begin{split} \widetilde{a}_{k,i} \det A[i,\alpha;i,\alpha] &= -\det A[j,\alpha;i,\alpha] \left( \widetilde{a}_{k,j} + \frac{\det A[i,\alpha;j,i,\alpha'] \det A[\alpha,k;i,\alpha]}{\det A[r,\alpha';i,\alpha']} \right) \\ &+ \frac{\det A[j,\alpha;j,i,\alpha'] \det A[\alpha,k;i,\alpha] \det A[i,\alpha;i,\alpha]}{\det A[r,\alpha';i,\alpha']} \\ &= -\widetilde{a}_{k,j} \det A[j,\alpha;i,\alpha] - \frac{\det A[\alpha,k;i,\alpha]}{\det A[r,\alpha';i,\alpha']} \Big( \det A[i,\alpha;j,i,\alpha'] \\ &\times \det A[j,\alpha;i,\alpha] - \det A[j,\alpha;j,i,\alpha'] \det A[i,\alpha;i,\alpha] \Big) \\ &= -\widetilde{a}_{k,j} \det A[j,\alpha;i,\alpha] - \widetilde{a}_{k,k} \det A[k,\alpha;i,\alpha]. \quad \Box \end{split}$$

It is important to point out that, via permutation similarity, the labelling of the tree, per se, is not important. If the conjecture were correct for one labelling of a given tree, it would be correct for another. Indeed, it is an easy exercise to see that if a path is labelled in some other way than consecutively, a T-TP matrix still has the "last" eigenvector signed according to the alternatively labelled path.

Once the next three Lemmata are proven, Theorem 4 follows. In the first lemma we prove the statement of the theorem for any two pendent vertices. If the tree is not a path, then it has at least 3 pendent vertices. Then we prove the statement of the theorem assuming i is pendent and j is any vertex, and in the last lemma we prove the statement of the theorem to the theorem without assuming i and j are non-pendent vertices.

We are going to prove these Lemmata by induction on the number of vertices  $n, n \ge 2$ , of the tree T. The cases  $2 \le n \le 4$  were proven in [1], so we will assume  $n \ge 4$  and that T is not a path (in which case the claim is inmediate). Recall that  $\sigma$  is signed according to T. Then, we need to prove

$$\operatorname{sign}(\det A(i;j)) = (-1)^{i+j} \sigma_i \sigma_j, \tag{2}$$

for all  $1 \leq i, j \leq n$ . Note that if (2) holds, since

 $\operatorname{sign}(\det A(i;j)) = (-1)^{i+j} \sigma_i \sigma_j \iff \operatorname{sign}(\widetilde{a}_{i,j}) = \sigma_i \sigma_j$ 

the matrix

$$\operatorname{diag}(\sigma_1,\cdots,\sigma_n) A \operatorname{diag}(\sigma_1,\cdots,\sigma_n)$$

is entry-wise positive.

**Lemma 8.** Under the same assumptions as in Theorem 4, for any two different pendent vertices  $p_1$  and  $p_2$ ,

$$sign(\det A(p_1; p_2)) = (-1)^{p_1 + p_2} \sigma_{p_1} \sigma_{p_2}.$$

**Proof.** Since after removing a pendent vertex of a tree it is still a tree (the tree has at least 4 vertices and it is not a path), we can apply the induction hypothesis to obtain

$$\det A(p_1; p_2) = \det A[N_{p_1}, N_{p_2}] = (-1)^{p_1 + p_2 - 1} \det A[p_2, N_{p_1, p_2}; p_1, N_{p_1, p_2}]$$

Without loss of generality, let  $p_3$  be the last pendent vertex in N, with  $p_3 > \max\{p_1, p_2\}$ . Therefore, if we denote  $N_{p_1, p_2, p_3} \cup \{p_3\}$  by  $\alpha$  and use Sylvester's identity we get that  $(-1)^{p_1+p_2} \det A(p_1; p_2)$  is equal to

$$\frac{\det A[p_2,\alpha';\alpha] \det A[\alpha;p_1,\alpha'] - \det A[p_2,\alpha';p_1,\alpha'] \det A[\alpha;\alpha]}{\det A[\alpha';\alpha']}$$

Notice that since the tree, which is not a path, has at least 3 pendent vertices, we have rearranged the entries of  $\alpha$  in such a way that the last element of  $\alpha$  is the pendent vertex  $p_3$ , i.e.,  $\alpha' \cup \{p_3\} = \alpha$ ; while, for example,  $\tilde{a}_{p_1,p_2}|_{p_3}$  represents the entry  $(p_1, p_2)$  of the adjoint of the  $(n-1) \times (n-1)$  submatrix of A from which the  $p_3$ -th row and  $p_3$ -th column are removed. By the induction hypothesis sign(det  $A(p_3)(p_2; p_1)) = (-1)^{p_1+p_2} \sigma_{p_1} \sigma_{p_2}$ .

Here the denominator is positive because A is pendent-P and  $p_3$  is a pendent vertex; the numerator has the desired sign since (let us assume, for example, that  $p_1 < p_2$ )

$$\operatorname{sign}(\det A[p_2, \alpha'; \alpha]) = (-1)^{p_3} \sigma_{p_2} \sigma_{p_3},$$
$$\operatorname{sign}(\det A[\alpha; p_1, \alpha']) = (-1)^{p_3} \sigma_{p_1} \sigma_{p_3},$$
$$\operatorname{sign}(\det A[p_2, \alpha'; p_1, \alpha']) = -\sigma_{p_1} \sigma_{p_2},$$
$$\operatorname{sign}(\det A[\alpha; \alpha]) = +.$$

Observe that if  $p_1 < p_2$  and due to the re-labeling after the deleting of  $p_2$  in the new tree there is a shift in the resulting sign of det  $A(p_2)(p_1; p_3)$ .

Then, since  $p_1$ ,  $p_2$ , and  $p_3$  are pendent vertices, again by the induction hypothesis, we have

$$\operatorname{sign}(\det A[p_2, \alpha'; \alpha] \det A[\alpha; p_1, \alpha']) = \sigma_{p_2} \sigma_{p_3} \sigma_{p_1} \sigma_{p_3} = \sigma_{p_2} \sigma_{p_1},$$

and

$$-\operatorname{sign}(\det A[p_2, \alpha'; p_1, \alpha']) = \sigma_{p_1} \sigma_{p_2}$$

so that the claim follows.  $\Box$ 

Next, by using Lemma 7, we are going to prove the following result:

**Lemma 9.** Under the same assumptions as in Theorem 4, for any pendent vertex p and for any  $i, 1 \le i \le N$ ,

$$\operatorname{sign}(\det A(i;p)) = (-1)^{i+p} \sigma_i \sigma_p.$$

**Proof.** If *i* is a pendent vertex,  $i \neq p$ , then the result follows from Lemma 8. If i = p then the result follows since *p* is a pendent vertex and by the pendent-*P* hypothesis relative to *T*, we have

$$\det A(p;p) = \det A(p) > 0, \quad \sigma_p \, \sigma_p > 0 \qquad \Rightarrow \quad \operatorname{sign}(\det A(p;p)) = \sigma_p \sigma_p.$$

On the other hand, if i is not a pendent vertex, then setting in Lemma 7 the vertex j as another pendent vertex, namely q, and k = p, we get

$$0 = \tilde{a}_{p,i} \det A[i, N_{i,q,p}; i, N_{i,q,p}] + \tilde{a}_{p,q} \det A[q, N_{i,q,p}; i, N_{i,q,p}] + \tilde{a}_{p,p} \det A[p, N_{i,q,p}; i, N_{i,q,p}].$$

Taking into account that p is a pendent vertex, by hypothesis and induction, we have

$$sign(\det A[q, N_{i,q,p}; i, N_{i,q,p}]) = -\sigma_q \sigma_i,$$
  

$$sign(\det A[p, N_{i,q,p}; i, N_{i,q,p}]) = -\sigma_p \sigma_i,$$

 $\widetilde{a}_{p,p} > 0$ , and  $\operatorname{sign}(\widetilde{a}_{p,q}) = \sigma_p \, \sigma_q$ . Therefore

$$\operatorname{sign}(\widetilde{a}_{p,q} \det A[q, N_{i,q,p}; i, N_{i,q,p}]) = -\sigma_p \,\sigma_i = \operatorname{sign}(\widetilde{a}_{p,p} \det A[p, N_{i,q,p}; i, N_{i,q,p}]),$$

and since p and q are pendent vertices we have that

$$\det A[i, N_{i,q,p}; i, N_{i,q,p}] = \det A(p)(q; q) > 0,$$

hence  $\operatorname{sign}(\widetilde{a}_{p,i}) = \sigma_i \sigma_p$ , and so that the claim follows.  $\Box$ 

For the last lemma we need to use *Jacobi's identity* [3, (0.8.4.1)]

$$\det A[\alpha;\beta] = (-1)^{p(\alpha,\beta)} \det A \ \det A^{-1}[N \setminus \beta; N \setminus \alpha], \tag{3}$$

where  $|\alpha| = |\beta|$ , and  $p(\alpha, \beta) = \sum_{i \in \alpha} i + \sum_{j \in \beta} j$ .

**Lemma 10.** Under the same assumptions as in Theorem 4, for any pair (i, j), neither of which is pendent,

$$\operatorname{sign}(\det A(i;j)) = (-1)^{i+j} \sigma_i \sigma_j.$$

**Proof.** We prove this by contradiction. If we assume that  $\operatorname{sign}(\det A(i; j)) \neq (-1)^{i+j} \sigma_i \sigma_j$ then  $\operatorname{sign}(\tilde{a}_{j,i}) \neq \sigma_i \sigma_j$ . Let p any pendant vertex. Then, on one hand, we have

$$\det \widetilde{A}[j,p;i,p] = \begin{vmatrix} \widetilde{a}_{j,i} & \widetilde{a}_{j,p} \\ \widetilde{a}_{p,i} & \widetilde{a}_{p,p} \end{vmatrix} = \widetilde{a}_{j,i}\widetilde{a}_{p,p} - \widetilde{a}_{j,p}\widetilde{a}_{p,i},$$

so that, by Lemmata 8 and 9, we get

$$\operatorname{sign}\left(\det \widetilde{A}[j,p;i,p]\right) = -\sigma_i \sigma_j$$

On the other hand, since det A > 0, applying *Jacoibi's identity* we have

$$\operatorname{sign}\left(\operatorname{det} \widetilde{A}[j, p; i, p]\right) = \operatorname{sign}\left((-1)^{i+j} \operatorname{det} A[N_{i,p}; N_{j,p}]\right)$$
$$= \operatorname{sign}\left((-1)^{i+j} \operatorname{det} A(p)(i; j)\right),$$

so that it is equal to, by the induction hypothesis,  $\sigma_i \sigma_j$  which is a contradiction. Hence the result follows.  $\Box$ 

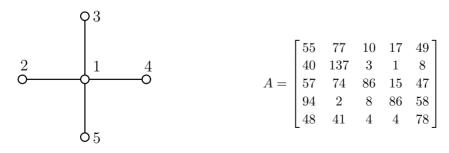
Theorem 4 follows from Lemmata 8, 9, and 10, as all types of minors are covered. As det(A) > 0, because of the relation between  $A^{-1}$  and  $\tilde{A}$ , Corollary 6 follows. Since the Perron root of  $A^{-1}$  is the reciprocal of the smallest absolute eigenvalue of A, that smallest eigenvalue is positive and has multiplicity 1. Because of the effect of similarity on eigenvectors (see [3]) the result about the signing of its eigenvector follows.

### 5. Remarks

We have shown that certain conditions on a matrix A, relative to a tree, are sufficient to reach the Neumaier conclusion. These conditions are more, see [1], than originally conjectured, but the originally conjectured conditions (T-TP) were not sufficient in general. We do not know if some of the additional hypotheses can be omitted. It is difficult to construct appropriate examples.

However, we do have some informative examples. It is possible for matrix A to be T-positive but have negative determinant and satisfy the Neumaier conclusion. We still do not know how common this is.

**Example 1.** For this example we have considered the 5-star and the following 5-by-5 matrix. It is easy to check that A is pendent-P relative to this tree and det(A) < 0.



Note that in this example, the eigenvector associated with the smallest eigenvalue,  $\lambda_5 \sim -0.23$ , has the predicted sign pattern. Here is the eigenvector in question, with each entry approximated to the nearest hundredth:

$$m{x} pprox egin{bmatrix} -2.3 \\ 0.6 \\ 0.15 \\ 1.8 \\ 1 \end{bmatrix}$$

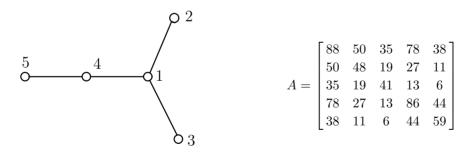
The adjoint of A is

$$\widetilde{A} = \begin{bmatrix} 70451860 & -27857784 & -4763560 & -11372966 & -30073840 \\ -18274672 & 7046528 & 1241168 & 2950496 & 7815680 \\ -4532012 & 1908264 & 18096 & 774494 & 2064504 \\ -55473260 & 21866360 & 3770144 & 8668470 & 23888344 \\ -30671880 & 12220096 & 2084744 & 4963592 & 12765448 \end{bmatrix}$$

Both  $\boldsymbol{x}$  and  $\widetilde{A}$  have the predicted sign pattern.

However, if A is T-TP but not pendent-P relative to T, the Neumaier conclusion may fail.

**Example 2.** (See [1].) For this example we have considered the following tree with 5 vertices and the following 5-by-5 matrix. It is easy to check that  $\det A(5) < 0$  therefore A is not pendent-P relative to this tree, and  $\det(A) < 0$ .



Here the eigenvector associated with the smallest eigenvalue,  $\lambda_5 \approx -2.54$ , does not have the predicted sign pattern. The following is the eigenvector in question, with each entry approximated to the nearest hundredth:

$$x \approx \begin{bmatrix} -68.08\\ 32.75\\ 26.69\\ 45.57\\ 1 \end{bmatrix}$$

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