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The maximum four point condition matrix of a tree



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ABSTRACT

The Four point condition (4PC henceforth) is a well known condition characterising distances in trees T. Let w, x, y, z be four vertices in T and let $d_{x,y}$ denote the distance between vertices x, y in T. The 4PC condition says that among the three terms $d_{w,x} + d_{y,z}$, $d_{w,y} + d_{x,z}$ and $d_{w,z} + d_{x,y}$ the maximum value equals the second maximum value. We define an $\binom{n}{2} \times \binom{n}{2}$ sized matrix Max4PC_T from a tree T where the rows and columns are indexed by size-2 subsets. The entry of Max4PC_T corresponding to the row indexed by $\{w, x\}$ and column $\{y, z\}$ is the maximum value among the three terms $d_{w,x} + d_{y,z}, d_{w,y} + d_{x,z}$ and $d_{w,z} + d_{x,y}$. In this work, we determine basic properties of this matrix like rank, give an algorithm that outputs a family of bases, and find the determinant of Max4PC_T when restricted to our basis.

We further determine the inertia and the Smith Normal Form

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(SNF) of Max4PC_T.

1. Introduction

Let T = (V, E) be a tree on n vertices. Associated to T are several matrices whose entries are functions of distance between the vertices. The most well studied of these is the $n \times n$ distance matrix D_T of T whose rows and columns are indexed by vertices of T. The (i, j)-th entry of D_T is $d_{i,j}$, the distance between vertex i and vertex j in T. About fifty years ago, Graham and Pollak in [13] showed that the determinant of D_T is independent of the structure of the tree T and only depends on n, the number of vertices in T. This result has inspired several generalizations (see for example [3–9,12,14,15]). These papers illustrate the wealth of results concerning distances in trees. We refer the reader to the book [2] by Bapat for a good introduction to such matrices. An important condition characterising distances in trees was given by Buneman in [11] and is called the *four-point condition* (henceforth denoted as 4PC).

Fix a tree T and denote the distance between vertices x, y in T as $d_{x,y}$. The 4PC states that for any four vertices w, x, y and z in T, among the three terms $d_{w,x} + d_{y,z}$, $d_{w,y} + d_{x,z}$ and $d_{w,z} + d_{x,y}$, the maximum value equals the second maximum value. In order to understand the 4PC in more detail, Bapat and Sivasubramanian in [10] studied the $\binom{n}{2} \times \binom{n}{2}$ matrix M_T whose rows and columns are indexed by pairs of distinct vertices. The entry in the row indexed by $\{w, x\}$ and column $\{y, z\}$ of M_T equals the minimum value among the three terms $d_{w,x} + d_{y,z}$, $d_{w,y} + d_{x,z}$ and $d_{w,z} + d_{x,y}$. They showed the surprising result that the rank of M_T is independent of the structure of T and only depends on n, the number of vertices in T. Among other results, they also gave the Smith Normal Form (henceforth SNF) of M_T . It is somewhat surprising that D_T , the distance matrix of T and M_T , the min-4PC matrix of T have the same rank and the same invariant factors. We term the matrix M_T as the minimum 4PC matrix and also denote it as Min4PC_T. Analogously, in this work, we define Max4PC_T, the $\binom{n}{2} \times \binom{n}{2}$ maximum 4PC matrix whose rows and columns are indexed by pairs of distinct vertices. The entry in the row indexed by $\{w, x\}$ and column $\{y, z\}$ of Max4PC_T equals the maximum value among the three terms $d_{w,x} + d_{y,z}$, $d_{w,y} + d_{x,z}$ and $d_{w,z} + d_{x,y}$.

Related to this, Azimi and Sivasubramanian in [1] studied the 2-Steiner distance matrix $\mathfrak{D}_2(T)$. This is also an $\binom{n}{2} \times \binom{n}{2}$ matrix with the entry in the row indexed by $\{w, x\}$ and column indexed by $\{y, z\}$ being the number of edges in a minimum subtree of T that contains the vertices w, x, y and z. For all positive integers k, one can define k-Steiner distance matrices $\mathfrak{D}_k(T)$ and in [1], the authors show that when k = 1, $\mathfrak{D}_1(T) = D_T$ is the usual distance matrix. Interestingly, in [1, Lemma 4] they showed that $\mathfrak{D}_2(T) = \frac{1}{2} \left(\operatorname{Max4PC}_T + \operatorname{Min4PC}_T \right)$. Thus, for any tree T, each entry of $\operatorname{Max4PC}_T$ and $\operatorname{Min4PC}_T$ have the same parity and their average is the corresponding entry of $\mathfrak{D}_2(T)$.

Thus, three $\binom{n}{2} \times \binom{n}{2}$ matrices are associated to a tree T: the maximum 4PC matrix (denoted Max4PC_T), the minimum 4PC matrix (denoted Min4PC_T) and the average 4PC matrix (denoted as $\mathfrak{D}_2(T)$). Among these three matrices, results are known for two matrices. See Bapat and Sivasubramanian [10] for results on Min4PC_T and see Azimi and Sivasubramanian [1] for results on $\mathfrak{D}_2(T)$. To the best of our knowledge, there are

no results on the third matrix, $Max4PC_T$. In this paper, we start filling this gap and study $Max4PC_T$ for a tree T. Our first result about $Max4PC_T$ is the following.

Theorem 1. Let T be a tree on $n \ge 3$ vertices having p pendant vertices. Then,

$$\operatorname{rank}(\operatorname{Max4PC}_T) = 2(n-p).$$

For a matrix M, let P, Q be subsets of the row and column indices respectively. By M(P, Q) we denote the submatrix of M obtained by deleting the rows in P and columns in Q. By M[P, Q] we denote the submatrix of P obtained by restricting M to the rows in P and the columns in Q.

We determine a class of bases \mathfrak{B} of the row space of $\operatorname{Max4PC}_T$ and for each $B \in \mathfrak{B}$, we determine the determinant of the submatrix $\operatorname{Max4PC}_T[B, B]$ of $\operatorname{Max4PC}_T$ induced on the rows and columns in B. Our basis B is constructed using a depth-first search type traversal of T. Our algorithm depends on a starting leaf vertex, and there are further choices as well in the execution of our algorithm. Thus, our output basis B will depend on these choices and is hence not unique. Nonetheless, the determinant of $\operatorname{Max4PC}_T$ when restricted to the rows and columns of all such constructed bases has a clean formula which is our next result.

Theorem 2. Let B be a basis for the row space of $Max4PC_T$ that is output by the algorithm described in Lemma 9. Then,

det Max4PC_T[B, B] =
$$(-1)^{n-p} 2^{2(n-p-1)}$$
.

As mentioned earlier, the invariant factors and hence the SNF of Min4PC_T were found by Bapat and Sivasubramanian in [10, Theorem 2]. As a counterpart, in Theorem 5, we determine the SNF of Max4PC_T. In [1, Theorem 18], the authors showed that $\mathfrak{D}_2(T)$ has exactly one positive eigenvalue, 2n - p - 2 negative eigenvalues and the rest of its eigenvalues are 0. If we denote the inertia of a real, symmetric matrix M by the triple (n_0, n_+, n_-) , where n_0 is the nullity of M, n_+ is the number of positive eigenvalues and n_- is the number of negative eigenvalues, then $\mathfrak{D}_2(T)$ has inertia $(\binom{n}{2} - 2n + p + 1, 1, 2n - p - 2)$. In Theorem 13, we determine the inertia of Max4PC_T and show that it has n - p

positive eigenvalues and n-p negative eigenvalues. Thus Theorem 13 refines Theorem 1 by giving the number of positive and negative eigenvalues.

2. Rank of $Max4PC_T$

Towards proving Theorem 1, we start with the following lemmas. For four vertices $u, v, w, x \in V(T)$, denote by $Max4PC_T(\{u, v\}, \{w, x\})$ the entry of $Max4PC_T$ indexed by the row $\{u, v\}$ and column $\{w, x\}$. Further, we denote the path between vertices u, v in T as the u-v path.

Lemma 3. Let T be a tree on n vertices. Suppose n is a pendant vertex of T with a unique neighbour n - 1. Let u be a vertex of T other than n and n - 1. Then, for all unordered pairs of distinct vertices $\{i, j\}$, we have

$$Max4PC_T(\{u, n\}, \{i, j\}) = Max4PC_T(\{u, n-1\}, \{i, j\}) + 1.$$

Proof. Recall that $u \neq n-1, n$. Therefore, when $v \neq n$, the *v*-*n* path in *T* must contain the vertex n-1. Thus, we have

$$d_{v,n} = d_{v,n-1} + 1$$
 and hence $d_{u,n} = d_{u,n-1} + 1.$ (1)

Let $1 \leq i < j \leq n$. Then by the definition of Max4PC_T, we have

$$\operatorname{Max4PC}_{T}(\{u,n\},\{i,j\}) = \max\{d_{u,n-1} + d_{i,j} + 1, \ d_{u,i} + d_{n,j}, \ d_{u,j} + d_{n,i}\}.$$
 (2)

We split the proof into two cases with the first case being when both $i \neq n$ and $j \neq n$. In this case, by (1) it follows that

$$Max4PC_T(\{u,n\},\{i,j\}) = max\{d_{u,n-1} + d_{i,j} + 1, \ d_{u,i} + d_{n-1,j} + 1, \ d_{u,j} + d_{n-1,i} + 1\}$$
$$= Max4PC_T(\{u,n-1\},\{i,j\}) + 1.$$

The second case is when exactly one of i, j equals n. Let j = n and hence $i \leq n - 1$. By the triangle inequality, we have

$$d_{u,n-1} + d_{i,n-1} \ge d_{u,i}$$
 and $d_{u,n} + d_{i,n} > 1 + d_{u,i}$. (3)

Therefore, by (3), we have

$$Max4PC_T(\{u, n\}, \{i, n\}) = max\{d_{u,n} + d_{i,n}, d_{u,i}\} = d_{u,n} + d_{i,n}$$

Further, note that

$$\begin{aligned} \operatorname{Max4PC}_{T}(\{u, n-1\}, \{i, n\}) \\ &= \max\{d_{u,n-1} + d_{i,n}, \ d_{u,i} + 1, \ d_{u,n} + d_{i,n-1}\} \\ &= \max\{d_{u,n} + d_{i,n} - 1, \ d_{u,i} + 1, \ d_{u,n} + d_{i,n} - 1\} \quad [by (1)] \\ &= d_{u,n} + d_{i,n} - 1 \qquad \qquad [by (1) \text{ and } (3)] \\ &= \operatorname{Max4PC}_{T}(\{u, n\}, \{i, n\}) - 1. \end{aligned}$$

This completes the proof. \Box

Lemma 4. Let T be a tree on n vertices. Suppose $p, q \in V(T)$ such that p is a pendant vertex of T with q being the quasi-pendant vertex adjacent to p. Let $u \in V(T)$ be a



Fig. 1. Illustrating Lemma 4.

neighbour of q other than p and B_u be the connected component of T - q that contains the vertex u (Fig. 1). Then,

$$Max4PC_{T}(\{p,q\},\{i,j\}) = \begin{cases} Max4PC_{T}(\{u,q\},\{i,j\}) + 2 & if \ i, j \in B_{u} \\ Max4PC_{T}(\{u,q\},\{i,j\}) & otherwise. \end{cases}$$

Proof. Clearly, for each $i \in T$ and $j \in B_u$, it follows by triangle inequality that

$$d_{i,j} < d_{u,i} + d_{q,j}.$$
 (4)

Let us first assume $i, j \in B_u$. Clearly $d_{p,v} = d_{u,v} + 2$ for each $v \in B_u$. Therefore, it follows that

$$\begin{aligned} \operatorname{Max4PC}_{T}(\{p,q\},\{i,j\}) &= \max\{d_{p,q} + d_{i,j}, \ d_{p,i} + d_{q,j}, \ d_{p,j} + d_{q,i}\} \\ &= \max\{1 + d_{i,j}, \ d_{u,i} + d_{q,j} + 2, \ d_{u,j} + d_{q,i} + 2\} \\ &= \max\{1 + d_{i,j}, d_{u,i} + d_{q,j}, \ d_{u,j} + d_{q,i}\} + 2 \end{aligned} \qquad [by (4)] \\ &= \max\{d_{u,q} + d_{i,j}, \ d_{u,i} + d_{q,j}, \ d_{u,j} + d_{q,i}\} + 2 \\ &= \operatorname{Max4PC}_{T}(\{u,q\},\{i,j\}) + 2. \end{aligned}$$

In the third last line above, we have used the easy to prove inequality that $1 + d_{i,j}$ is smaller than both $d_{u,i} + d_{q,j}$ and $d_{u,j} + d_{q,i}$. We now assume that $i \notin B_u$ and $j \in T$. Note that if i = p and $j \in T - p$ then $d_{p,j} + d_{u,q} = d_{q,j} + d_{p,u}$. It follows that

$$\begin{aligned} \operatorname{Max4PC}_{T}(\{p,q\},\{p,j\}) \\ &= \max\{d_{p,q} + d_{p,j}, \ d_{p,p} + d_{q,j}, \ d_{p,j} + d_{p,q}\} \\ &= \max\{d_{u,q} + d_{p,j}, \ d_{p,j} + d_{q,u}\} \\ &= \max\{d_{u,q} + d_{p,j}, \ d_{p,u} + d_{q,j}, \ d_{p,j} + d_{q,u}\} \\ &= \max\{d_{u,q} + d_{p,j}, \ d_{p,u} + d_{q,j}, \ d_{p,j} + d_{q,u}\} \\ &= \operatorname{Max4PC}_{T}(\{u,q\},\{p,j\}). \end{aligned}$$

We split the remaining part of the proof into two cases with the first case being when $i \notin B_u \cup \{p\}$ and $j \in B_u$. Clearly, in this case, $d_{i,j} = d_{i,q} + d_{q,u} + d_{u,j}$, and so we get

$$d_{u,i} + d_{q,j} = d_{i,j} + 1 > d_{u,j} + d_{q,i} = d_{i,j} - 1.$$
(5)

Therefore, we have

$$\begin{aligned} \operatorname{Max4PC}_{T}(\{p,q\},\{i,j\}) &= \max\{1 + d_{i,j}, \ d_{u,i} + d_{q,j}, \ d_{u,j} + 2 + d_{q,i}\} & \text{[as } d_{p,i} = d_{u,i}] \\ &= \max\{d_{u,q} + d_{i,j}, \ d_{u,i} + d_{q,j}, \ d_{u,j} + d_{q,i}\} & \text{[by (5)]} \\ &= \operatorname{Max4PC}_{T}(\{u,q\},\{i,j\}). \end{aligned}$$

Our second case, is when $i \notin B_u \cup \{p\}$ and $j \notin B_u$.

Note that if $j \neq p$ then $d_{p,i} = d_{u,i}$, $d_{p,j} = d_{u,j}$ and so it follows that

$$Max4PC_T(\{p,q\},\{i,j\}) = max\{d_{u,q} + d_{i,j}, d_{u,i} + d_{q,j}, d_{u,j} + d_{q,i}\}$$
$$= Max4PC_T(\{u,q\},\{i,j\})$$

Finally, let us assume j = p and so $i \notin B_u \cup \{p\}$. Clearly, $d_{p,i} = d_{u,i}$. Therefore, we get

$$\begin{aligned} \operatorname{Max4PC}_{T}(\{p,q\},\{i,p\}) &= \max\{d_{p,q} + d_{i,p}, \ d_{p,i} + d_{q,p}, \ d_{p,p} + d_{q,i}\} \\ &= \max\{d_{u,q} + d_{i,p}, \ d_{p,i} + d_{q,p}\} \\ &= \max\{d_{u,q} + d_{i,p}, \ d_{q,i} + d_{u,p}, \ d_{u,i} + d_{q,p}\} \\ &= \operatorname{Max4PC}_{T}(\{u,q\},\{i,p\}). \end{aligned}$$
 [as $d_{q,i} < d_{p,i}$]

This completes the proof. \Box

With the two lemmas above, we are now ready to prove our main result of this section.

Proof. (Of Theorem 1) We use induction on n, the number of vertices in the tree T. When n = 3, the only tree is P_3 , the path on three vertices. It can be easily verified that $Max4PC_{P_3} = \begin{bmatrix} 2 & 3 & 2 \\ 3 & 4 & 3 \\ 2 & 3 & 2 \end{bmatrix} \text{ and } rank(Max4PC_{P_3}) = 2. \text{ Therefore, the result is true for}$ all trees on three vertices

Assume that the result is true for all trees on n-1 vertices. Let T be a tree on n vertices. Without loss of any generality, let n be a pendant vertex that is adjacent to n-1. Let \widehat{T} be the tree obtained by deleting the vertex n from T. We divide the proof into two cases based on the degree of vertex n-1 in T.

Case I: There exists a quasi-pendant vertex with degree two. We relabel the vertices of T if necessary. We assume that n is a leaf of T adjacent to n-1 and that n-1 has degree 2. Let n, n-2 be the two neighbours of n-1. Let \widehat{T} be the tree obtained from T by deleting the vertex n from T.

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Let \mathbb{V}_n be the collection of all 2-size unordered subsets of $[n] := \{1, 2, ..., n\}$ with distinct elements and let $\mathbb{U}_{n-1} = \{\{i, n\} : i \in [n-1]\}$. We order the elements of \mathbb{V}_n as $\mathbb{V}_n = (\mathbb{V}_{n-1}, \mathbb{U}_{n-1})$ and use this order of pairs to index rows and columns of Max4PC_T. We thus write Max4PC_T in partitioned form as

$$\mathrm{Max4PC}_{T} = \begin{bmatrix} \mathrm{Max4PC}_{\widehat{T}} & \mathrm{Max4PC}_{12} \\ \mathrm{Max4PC}_{12}^{t} & \mathrm{Max4PC}_{22} \end{bmatrix},$$

where $\operatorname{Max4PC}_{12} = \operatorname{Max4PC}_{T}[\mathbb{V}_{n-1}, \mathbb{U}_{n-1}]$ and $\operatorname{Max4PC}_{22} = \operatorname{Max4PC}_{T}[\mathbb{U}_{n-1}, \mathbb{U}_{n-1}]$.

For a pair $\{u, v\}$ of distinct vertices in V, denote the row (column) of Max4PC_T indexed by $\{u, v\}$ as $\operatorname{Row}_{u,v}$ (as $\operatorname{Col}_{u,v}$ respectively). We perform the following row and column operations. For $1 \leq i < n-1$, perform $\operatorname{Row}_{i,n} = \operatorname{Row}_{i,n} - \operatorname{Row}_{i,n-1}$ and also perform $\operatorname{Col}_{i,n} = \operatorname{Col}_{i,n} - \operatorname{Col}_{i,n-1}$. If performing row and column operations on M gives us the matrix N, we denote this by $M \sim N$. By Lemma 3, we get

$Max4PC_T \sim$	$\left\lceil \text{Max4PC}_{\widehat{T}} \right\rceil$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	u
	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	0	0 : 0 1
	u^t	$0 \cdots 0 1$	2

Denote the row indexed by $\{u, v\}$ in $\operatorname{Max4PC}_{\widehat{T}}$ as $\operatorname{Row}_{\widehat{T}}(u, v)$. In \widehat{T} , let vertex n-2 be adjacent to vertices n-1 and n-3. Note that we only need the degree of n-2 in \widehat{T} to be at least two, not exactly two. Since vertex n-1 is a pendant vertex in \widehat{T} , by Lemma 3, for all $v \in \widehat{T} - \{n-1, n-2\}$, we get $\operatorname{Row}_{\widehat{T}}(n-1, v) = \operatorname{Row}_{\widehat{T}}(n-2, v) + \mathbf{1}^t$.

Further, note that $\operatorname{Max4PC}_T(\{n-1,n\},\{n-1,n-3\}) = 3$ and $\operatorname{Max4PC}_T(\{n-1,n\},\{n-2,n-3\}) = 4$. Hence, by performing the row operation $\operatorname{Row}_{n-2,n} = \operatorname{Row}_{n-2,n-3}$ $\operatorname{Row}_{n-1,n-3} + \operatorname{Row}_{n-2,n-3}$ and $\operatorname{Col}_{n-2,n} = \operatorname{Col}_{n-2,n} - \operatorname{Col}_{n-1,n-3} + \operatorname{Col}_{n-2,n-3}$, we get

$$Max4PC_{T} \sim \begin{bmatrix} Max4PC_{\hat{T}} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{2} \\ \mathbf{0} & \mathbf{0} & \mathbf{2} & \mathbf{2} \end{bmatrix}$$

This completes the proof of case I.

Case II: All quasi-pendant vertices in T have degree at least three: Let (v_1, \ldots, v_k) be a path whose length is equal to the diameter of T. Clearly v_1 is a pendant vertex and v_2 is a quasi-pendant vertex in T. As all quasi pendant vertices have degree at least

three, v_2 has another pendant vertex p other than v_1 adjacent to it. By relabelling, we assume that $v_1 = n$ and p = n - 1 are two pendant vertices in T adjacent to $v_2 = n - 2$. Further, as n - 2 has degree at least three, let n - 3 be adjacent to n - 2. By Lemma 3,

$$\operatorname{Row}_{i,n} = \operatorname{Row}_{i,n-1} = \operatorname{Row}_{i,n-2} + \mathbf{1}^t$$
, for each $i \neq n-2$.

Let B_{n-3} be the connected component of $T - \{n-2\}$ that contains the vertex n-3. By Lemma 4, we get

$$\begin{aligned} \operatorname{Max4PC}_{T}(\{n-2,n\},\{i,j\}) \\ &= \begin{cases} \operatorname{Max4PC}_{T}(\{n-3,n-2\},\{i,j\}) + 2 & \text{if } i, j \in B_{n-3} \\ \operatorname{Max4PC}_{T}(\{n-3,n-2\},\{i,j\}) & \text{otherwise} \end{cases} \\ &= \operatorname{Max4PC}_{T}(\{n-2,n-1\},\{i,j\}), \quad \text{for each } 1 \leq i < j \leq n. \end{aligned}$$

Hence, by performing the row operation $\operatorname{Row}_{i,n} = \operatorname{Row}_{i,n} - \operatorname{Row}_{i,n-2} - \operatorname{Row}_{n-3,n-1} + \operatorname{Row}_{n-3,n-2}$ and $\operatorname{Col}_{i,n} = \operatorname{Col}_{i,n} - \operatorname{Col}_{i,n-2} - \operatorname{Col}_{n-3,n-1} + \operatorname{Col}_{n-3,n-2}$, when $i \neq n-2$ and $\operatorname{Row}_{n-2,n} = \operatorname{Row}_{n-2,n} - \operatorname{Row}_{n-2,n-1}$ and $\operatorname{Col}_{n-2,n} = \operatorname{Col}_{n-2,n} - \operatorname{Col}_{n-2,n-1}$ we get

$$Max4PC_T \sim \begin{bmatrix} Max4PC_{\widehat{T}} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{bmatrix}.$$

This completes the proof of case II. Our proof is complete. \Box

3. Smith normal form of $Max4PC_T$

In this section, we determine the invariant factors of $Max4PC_T$. Our main result is the following.

Theorem 5. Let T be a tree on $n \ge 3$ vertices with p leaves. Then, the invariant factors of Max4PC_T are

$$\underbrace{\underbrace{\binom{n}{2}-2(n-p)}_{0,\cdots,0}, 1, 1, \underbrace{2(n-p-1)}_{2,\cdots,2}}_{2,\cdots,2}.$$

Proof. We prove the result by induction on the number of vertices in the tree T. Our base case is when n = 3. In this case, the only tree is the path P_3 on three vertices. Clearly,

$$\operatorname{Max4PC}_{P_3} = \begin{bmatrix} 2 & 3 & 2 \\ 3 & 4 & 3 \\ 2 & 3 & 2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 2 & 3 & 2 \\ 3 & 4 & 3 \\ 0 & 0 & 1 \end{bmatrix}.$$

Therefore, the result follows when n = 3.

We assume that the result is true for all trees on n-1 vertices. Let T be a tree on n vertices where n > 3. Without loss of generality, let us assume that n is a pendant vertex adjacent to n-1. Let $\widehat{T} = T - \{n\}$ be the tree obtained by deleting the vertex n from T. As done earlier, we divide the proof into two cases based on the degree of vertex n-1 in T.

Case I: If the degree of n - 1 in T is two, then, as done in Case I of the proof of Theorem 1 we see that

$Max4PC_T \sim$	$\operatorname{Max4PC}_{\widehat{T}}$	0	0		$Max4PC_{\widehat{T}}$	0	0
	0	0	0		0	0	0
	0	0	2	\sim	0	0 -2	0
	0	0 2	2		0	0	2

The second similarity above is obvious and so our proof is over in this case.

Case II: If the degree of n-1 in T is at least three, then as done in Case II of the proof of Theorem 1 we see that

$$Max4PC_T \sim \begin{bmatrix} Max4PC_{\widehat{T}} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{bmatrix}$$

Hence, in both cases, the result follows by applying the induction hypothesis. \Box

4. Basis for the row space of $Max4PC_T$

In this section we define a set \mathfrak{B} of bases of the row space of Max4PC_T. We start with the following Corollary about the rank of Max4PC_T when we remove a type of leaf from T.

Corollary 6. Let T be a tree on n vertices with n > 3. Suppose there exist two leaves u and v adjacent to the same vertex. Then we have

$$\operatorname{rank}(\operatorname{Max4PC}_T) = \operatorname{rank}(\operatorname{Max4PC}_{T-u}) = \operatorname{rank}(\operatorname{Max4PC}_{T-v}).$$

Proof. Follows from Theorem 1. \Box

Let T be a tree on n vertices with p leaves. By Theorem 1, the rank of $Max4PC_T$ is 2(n - p). To give a basis for the rowspace of $Max4PC_T$, we need an index set with cardinality 2(n - p). We know that the number of blocks in LG(T), the line graph of T is n - p. Thus, in order to construct a basis for RowSpace($Max4PC_T$) we shall take two elements from each block of LG(T) in the following algorithmic way. Our algorithm is very similar to a depth first search (DFS) algorithm. It turns out, that our algorithm is easy for non-star graphs and so we first handle the case when T is a star tree. **Lemma 7.** Let T be a star tree on n vertices. Then, the rank of Max4PC_T is two. Suppose 1 is the central vertex of T, then, the rows indexed by $\{1,i\}$ and $\{j,k\}$ are linearly independent, where $1 < i \leq j < k \leq n$. Further, let \mathfrak{B} be the collection $\{\{1,i\},\{j,k\}\}$ where $1 < i \leq j < k \leq n$. Let $B \in \mathfrak{B}$ be a basis. Then, the determinant of the sub-matrix Max4PC_T[B, B] of Max4PC_T induced on the rows and columns in B is given by

$$\det \operatorname{Max4PC}_T[B, B] = -1.$$

Proof. Let *T* be a star tree on *n* vertices and let 1 be its central vertex (having degree n-1). Thus $2, \ldots, n$ are leaves of *T*. Let \mathbb{V}_n be the collection of all 2-size subsets of [n], $\mathbb{V}_1 = \{\{1, i\} \mid 2 \leq i \leq n\}, \mathbb{V}_2 = \{\{j, k\} \mid 2 \leq j < k \leq n\}$. Clearly \mathbb{V}_n can be partitioned as $\mathbb{V}_1 \cup \mathbb{V}_2$. Thus, we write Max4PC_T in partitioned form as

$$\operatorname{Max4PC}_{T} = \begin{bmatrix} 2J_1 & 3J_2\\ 3J_2^t & 4J_3 \end{bmatrix},$$

where each J_i is an all ones matrix with appropriate size, i = 1, 2, 3. This completes the proof. \Box

Note that if T is a tree on three vertices then T is a star tree. Henceforth, we assume that T is a tree on at least four vertices, and that T is not a star tree.

Remark 8. Let T be a tree on $n \ge 3$ vertices and LG(T) be its line graph. Then, it is easy to see that the number of vertices in each block of LG(T) is at least two.

Lemma 9 (Algorithm to construct a basis for row space of Max4PC_T). Let T be a tree on n > 3 vertices and LG(T) be its line graph. Initialise G = LG(T) and $B = \emptyset$.

Suppose T is not a star tree. Consider a vertex $\{p,q\}$ in G where p is a leaf in T and q is adjacent to p. Set the vertex $\{p,q\}$ of LG(T) as a starting vertex and set the next starting vertex set as the empty set.

- Step 1. Note that the starting vertex cannot be a cut vertex of G. Therefore, there exists a unique block B_c in G that contains the starting vertex. We call the block B_c as the current block.
- Step 2. If the current block B_c contains a cut vertex of G.
 - a. We choose a cut vertex $\{u, v\}$ in B_c and call it the chosen vertex. Further, add all other cut vertices of G that are in B_c (that is, other than the cut vertex $\{u, v\}$) into the next starting vertex set.
 - b. Let Ĝ be the graph obtained from G by removing all edges of B_c and then deleting all the non-cut vertices of B_c from G. (Define G = G − {edges in B_c} and then define Ĝ = G − (B_c − {non cut vertices in B_c}). Thus, Ĝ has one block lesser than G.) Note that all the cut vertices of G which are in B_c become non-cut vertices in Ĝ. Set G = Ĝ.

- c. To our set B, we add two elements; the starting vertex and the symmetric difference between the starting vertex and the chosen vertex $\{u, v\}$.
- d. Redefine the starting vertex as the chosen vertex $\{u, v\}$ and go to Step 1.
- Step 3. If the current block B_c does not contain any cut vertex of G.
 - a. Choose a vertex $\{u, v\}$ in B_c other than the starting vertex and call it the chosen vertex.
 - b. Add the two elements starting vertex and the chosen vertex $\{u, v\}$ to B.
 - c. Define $\widehat{G} = G B_c$. Set $G = \widehat{G}$.
 - d. If next starting vertex set is the empty set, output B and terminate the algorithm. Otherwise, choose an element, say $\{w, x\}$ from the next starting vertex set, and delete it from next starting vertex set. Now redefine the starting vertex as $\{w, x\}$ and go to Step 1.

In the following example we illustrate the algorithm described in Lemma 9.

Example 10. Consider the tree T shown below. Its line graph LG(T) is shown on the right.



Suppose we start the algorithm by choosing the leaf 1 in T. Therefore, $\{1, 2\}$ is our *starting vertex*. We use black coloured, grey coloured, and red coloured nodes to represent the *starting vertex*, the *chosen vertex*, and the *next starting vertex* respectively.



Recall that initially G = LG(T). The block containing $\{1, 2\}$ is the current block B_c and is marked using dotted lines. Clearly, B_c contains only one other cut vertex of G

(vertex $\{2, 4\}$) and so the *chosen vertex* is $\{2, 4\}$. As there is only one cut vertex of G in B_c , by Step 2a, the *next starting vertex set* is the empty set (see the graph drawn on the left in the above diagram). By Step 2b, construct \hat{G} from G by deleting all edges of B_c along with vertices $\{1, 2\}$ and $\{2, 3\}$. (See the graph drawn on the right in the above diagram.) By Step 2c, add $\{1, 2\}$ and $\{1, 4\}$ (the symmetric difference of $\{1, 2\}$ and $\{2, 4\}$) to B. By Step 2d, we make $\{2, 4\}$ as the current *starting vertex* and proceed to Step 1.



As the starting vertex is $\{2, 4\}$, the block that contains it is B_c . Note that B_c contains two cut vertices of G: viz $\{4, 5\}$ and $\{4, 8\}$. By Step 2a, we choose $\{4, 8\}$ as our *chosen* vertex and so the next starting set is $\{\{4, 5\}\}$. (See the left graph in the above diagram.) Construct \widehat{G} from G by performing Step 2b. \widehat{G} is shown in the graph on the right, in the above diagram. By Step 2c, after adding $\{2, 4\}$ and $\{2, 8\}$ (the symmetric difference of $\{2, 4\}$ and $\{4, 8\}$) to B, the set B becomes $B = \{\{1, 2\}, \{1, 4\}, \{2, 4\}, \{2, 8\}\}$. By Step 2d, we make $\{4, 8\}$ as the current starting vertex and proceed to Step 1 again.

As the starting vertex is $\{4, 8\}$, the current block B_c is the one containing it and is drawn with dotted lines. Note that B_c does not contain any cut vertex of G. By Step 3a, we choose $\{8, 9\}$ as our *chosen vertex*. (See the left graph in the below diagram.) By applying Step 3b, the set B now becomes $B = \{\{1, 2\}, \{1, 4\}, \{2, 4\}, \{2, 8\}, \{4, 8\}, \{8, 9\}\}$. Note that no symmetric difference is performed to the newly added elements of B at this stage. Construct \hat{G} from G by following Step 3c, which is shown in the right graph of the below diagram. Note that $\{4, 5\}$ is the only element on *next starting vertex set*. Thus, $\{4, 5\}$ is our *starting vertex* and we proceed to Step 1.





Fig. 2. Red coloured elements of LG(T) indicate elements contributed to B in Example 10. (For interpretation of the colours in the figure(s), the reader is referred to the web version of this article.)

Since $\{4,5\}$ is our starting vertex, by Step 1, the current block B_c is $\{\{4,5\}, \{5,6\}, \{5,10\}\}$. Note that B_c contains only one cut vertex of G which is our chosen vertex and is marked with grey coloured node in the below figure. By Step 2b, we construct the graph \hat{G} , see the right side graph in the below figure. After applying Step 2c, the set B becomes

 $B = \{\{1,2\},\{1,4\},\{2,4\},\{2,8\},\{4,8\},\{8,9\},\{4,5\},\{4,6\}\}.$

Now proceed to Step 1 again with $\{5, 6\}$ as our *starting vertex*.



Since $\{5, 6\}$ is starting vertex, by Step 1, the current block B_c is $\{\{5, 6\}, \{6, 7\}\}$. Note that B_c does not contain any cut vertex of G. After applying Steps 3a-b, the set B becomes

$$B = \{\{1,2\},\{1,4\},\{2,4\},\{2,8\},\{4,8\},\{8,9\},\{4,5\},\{4,6\},\{5,6\},\{6,7\}\}.$$

Note that by applying Step 3c, we will get an empty graph as \widehat{G} . Since there is no element in *next starting vertex set*, by Step 3d, we terminate the process. Note that the final set B contains 10 elements and each block of LG(T) contributes exactly two elements to B. We mark those elements of LG(T) using red colour in Fig. 2. Note that red coloured edges of LG(T) mean we take the symmetric difference of the end points of this edge to get a 2-sized subset of V(T).

Define \mathfrak{B} to be the union of all the sets *B* obtained by the algorithm described in Lemma 9 where the union is taken over all possible choices of starting vertices. In our next result, we discuss some properties of the output *B* obtained by applying the algorithm.

Theorem 11. Let T be a tree on $n \ge 3$ vertices with p leaves. Let $B \in \mathfrak{B}$ be an output of our algorithm described in Lemma 9. Then, the following is true.

- a. If T is not a star tree, then there exist unique vertices $u, v, w \in T$ such that $\{u, v\}, \{u, w\} \in B$ with d(u) = 1, d(w) > 1 (recall d(u) is the degree of vertex u) and with both $\{u, v\}, \{v, w\} \in E(T)$.
- b. The number of elements in B is 2(n-p).
- c. The set B is a basis for the row space of $Max4PC_T$.
- d. We have det Max4PC_T[B, B] = $(-1)^{n-p} 2^{2(n-p-1)}$.

Proof. Proof of Item a. In the algorithm, the initial starting vertex $\{u, v\}$ is clearly taken with u being a leaf adjacent to v. Since T is not a star, the number of blocks in LG(T) is at least two. Thus, the block of LG(T) that contains the vertex $\{u, v\}$ must contain a cut vertex of G. By Step 2 of Lemma 9, it follows that there exists a cut vertex $\{v, w\} \in LG(T)$ that give rise to $\{u, v\}, \{u, w\} \in B$.

We now show the uniqueness of u. Suppose, to the contrary, there are $u_1, v_1, w_1 \in T$ such that $\{u_1, v_1\}, \{u_1, w_1\} \in B$ with $u \neq u_1, \{u_1, v_1\}$ and $\{v_1, w_1\} \in E(T)$, with $d(u_1) = 1$, and $d(w_1) > 1$. Clearly, both $\{u_1, v_1\}, \{u_1, w_1\}$ were added to B in Step 2c. Since $\{u_1, w_1\}$ is not an edge in T, it follows that in some step $\{u_1, v_1\}$ was a starting vertex. As $u \neq u_1$, it follows that degree of the vertex u_1 in T is at least two. This contradicts that u_1 is a leaf.

Proof of Item b. If T is a star tree, then, there is nothing to prove. Suppose T is not a star tree. By Lemma 9, note that in each step, exactly one block of the line graph of T is removed and exactly two elements corresponding to that block are added in B. Since the number of block in LG(T) is (n-p), B has 2(n-p) elements.

Proof of Item c. We use induction on n. Our base case when T has three vertices can easily be verified. Suppose the result is true for all tree on n-1 vertices. Let T be a tree on n vertices. If T is a star tree then the result follows by Lemma 7.

Suppose T is not a star tree. Let B be a set output by our algorithm described in Lemma 9. By part (a), there exist unique vertices u, v, w in B such that $\{u, v\}, \{u, w\} \in T$ with d(u) = 1 and $\{u, v\}, \{v, w\} \in E(T)$. Without of loss of generality let us assume u = 1, v = 2, and w = 3. Note that, by Lemma 3, we get

$$Max4PC_T[B, \{1, 3\}] = Max4PC_T[B, \{2, 3\}] + 1.$$
(6)

Now note that for each leaf $l \neq 1$ in T, if $\{l, v\} \in B$ for some v then $\{v, l\} \in E(T)$ and $\{v, w\} \in B$, where w is a neighbour of v other than l. Without loss of any generality, let us assume x is a leaf lying on a path whose length is the diameter of T with $\{x, y\} \in E(T)$. Note that if there is more than one leaf attached at y, then by the induction hypothesis and Corollary 6, it follows that B is a basis for the row space of Max4PC_T.

Let us assume d(y) = 2 and $\{y, z\} \in E(T)$. It follows that $\{x, y\}, \{y, z\} \in B$. Suppose w be the neighbour of z other than y such that $\{z, w\} \in B$. Let \widehat{B} be the set obtained by

applying Lemma 9 on T-x in the same sequence as it was applied for T while obtaining the set B. By induction hypothesis, \hat{B} is a basis for the row space of Max4PC_{T-x}. Now we divide the remaining part of the proof into two cases.

We first assume that $\{y, z\} \in \widehat{B}$. It follows that $\{y, w\} \in B$. Then, $\widehat{B} = B \setminus \{\{x, y\}, \{y, w\}\}$. Note that the matrix Max4PC_T[B, B] can be partitioned as

$$\begin{cases} \{x,y\} & \{y,w\} \\ \\ \operatorname{Max4PC}_{T}[B,B] = & \{x,y\} \\ & \{y,w\} \end{cases} \begin{bmatrix} \operatorname{Max4PC}_{T-x}[\widehat{B},\widehat{B}] & \boldsymbol{u} & \boldsymbol{v} \\ & \boldsymbol{u}^{t} & 2 & 3 \\ & \boldsymbol{v}^{t} & 3 & 4 \end{bmatrix}$$

where $\boldsymbol{u} = \text{Max4PC}_T[\widehat{B}, \{x, y\}]$ and $\boldsymbol{v} = \text{Max4PC}_{T-x}[\widehat{B}, \{y, w\}].$

By Lemma 3, we have

$$\operatorname{Max4PC}_{T-x}[\widehat{B}, \{y, w\}] = \operatorname{Max4PC}_{T-x}[\widehat{B}, \{z, w\}] + \mathbf{1}.$$

Further, note that $\operatorname{Max4PC}_T(\{z, w\}, \{x, y\}) = 4$ and $\operatorname{Max4PC}_T(\{z, w\}, \{y, w\}) = 3$. Hence, by performing the row operation $\operatorname{Row}_{y,w} = \operatorname{Row}_{y,w} - \operatorname{Row}_{z,w} - (\operatorname{Row}_{1,3} - \operatorname{Row}_{2,3})$ in $\operatorname{Max4PC}_T[B, B]$ and an identical column operation, we obtain

		$\{x, y\}$	$\{y, w\}$
	$\operatorname{Max4PC}_{T-x}[\widehat{B},\widehat{B}]$	$oldsymbol{u}$	0]
$\{x, y\}$	$oldsymbol{u}^t$	2	-2
$\{y, w\}$	0^t	-2	0

It follows that det Max4PC_T[B, B] = $(-4) \times \det \operatorname{Max4PC}_{T-x}[\widehat{B}, \widehat{B}]$. Hence, by induction hypothesis, it follows that B is a basis for the row space of Max4PC_T.

Now we consider the case when $\{y, z\} \notin \widehat{B}$. It follows that $\widehat{B} = B \setminus \{\{y, z\}, \{x, y\}\}$. We can clearly partition the matrix Max4PC_T[B, B] as follows.

$$\begin{cases} \{y, z\} & \{x, y\} \\ \text{Max4PC}_T[B, B] = & \{y, z\} \\ & \{x, y\} \end{cases} \begin{bmatrix} \text{Max4PC}_{T-x}[\widehat{B}, \widehat{B}] & \boldsymbol{w} & \boldsymbol{u} \\ & \boldsymbol{w}^t & 2 & 2 \\ & \boldsymbol{u}^t & 2 & 2 \\ & \boldsymbol{u}^t & 2 & 2 \\ \end{cases},$$

where $\boldsymbol{u} = \text{Max4PC}_{T-x}[\widehat{B}, \{x, y\}]$ and $\boldsymbol{w} = \text{Max4PC}_T[\widehat{B}, \{y, z\}].$

By Lemma 4, it follows that u = w + 21. Hence, by performing the row operation Row_{x,y} = Row_{x,y} - Row_{y,z} - (Row_{1,3} - Row_{2,3}) in Max4PC_T[B, B] and an identical column operation, we get

$$\begin{cases} \{y,z\} & \{x,y\} \\ \\ \{y,z\} \\ \{x,y\} \\ \end{bmatrix} \begin{bmatrix} \operatorname{Max4PC}_{T-x}[\widehat{B},\widehat{B}] & \boldsymbol{u} & \boldsymbol{0} \\ \boldsymbol{u}^t & 2 & -2 \\ \boldsymbol{0}^t & -2 & 0 \end{bmatrix}$$

It follows that det Max4PC_T[B, B] = (-4) × det Max4PC_{T-x}[\hat{B}, \hat{B}]. Hence, by the induction hypothesis, it follows that B is a basis for the row space of Max4PC_T, completing the proof.

Proof of Item d. The result follows from the proof of Item c and noting that when n = 3, the determinant value is (-1). \Box

5. Inertia of $Max4PC_T$

In this section, we determine the inertia of Max4PC_T. For an $n \times n$ real symmetric matrix A, we denote its number of positive, negative and zero eigenvalues by n_+ , n_- and n_0 , respectively. We denote the inertia of A by Inertia(A) and define it as the triple (n_0, n_+, n_-) . Since A is a real symmetric matrix, $n_0 + n_+ + n_- = n$. We recall the well known Sylvester's law of inertia.

Theorem 12 (Sylvester's Law of Inertia). Let A be a real symmetric matrix of order n and let Q be a nonsingular matrix of order n. Then $Inertia(A) = Inertia(QAQ^t)$.

The main result of this Section is the following where we determine the inertia of $Max4PC_T$.

Theorem 13. Let T be a tree on n vertices with p leaves. Then, the inertia of $Max4PC_T$ is

Inertia(Max4PC_T) =
$$(n_0, n_+, n_-) = \left(\binom{n}{2} - 2(n-p), n-p, n-p\right).$$

Proof. By induction on n, we first prove that if B is a basis for the row space of Max4PC_T obtained by applying Lemma 9 then Inertia(Max4PC_T[B, B]) = (0, n - p, n - p).

If T is tree on n < 4 vertices then the result can be verified easily. Now notice that if two leaves u and v of T have a common neighbour, then by Corollary 6, we have

$$\operatorname{rank}(\operatorname{Max4PC}_{T}) = \operatorname{rank}(\operatorname{Max4PC}_{T-u}) = \operatorname{rank}(\operatorname{Max4PC}_{T-v}).$$

Hence, the result follows by applying induction hypothesis on the tree T - u. We thus assume that T is a tree such that every quasi-pendant vertex of T is adjacent to exactly one leaf. Let B be a basis of the row space of Max4PC_T obtained by applying Lemma 9.

Without loss of generality, assume that n is a leaf adjacent to n-1 with $\{n, n-1\} \in B$ but $\{n, n-2\} \notin B$ where n-2 is a neighbour of n-1. We first compute

Inertia(Max4PC_T[B, B]). The proof of Item c of Theorem 11 gives det Max4PC_T[B, B] = $-4 \det \operatorname{Max4PC}_{T-n}[\widehat{B}, \widehat{B}]$, where \widehat{B} is the basis for the row space of Max4PC_{T-n} obtained by applying Lemma 9 on T-n in the same sequence as applied to get B.

Clearly, by Theorem 1, rank(Max4PC_T) = rank(Max4PC_{T-n}) + 2 and so the number of nonzero eigenvalues of Max4PC_T[B, B] is two more than of Max4PC_{T-n}[\hat{B}, \hat{B}]. Since the product of det Max4PC_T[B, B] and det Max4PC_{T-n}[\hat{B}, \hat{B}] is negative, the number of positive eigenvalues of Max4PC_T[B, B] is exactly one more than that of Max4PC_{T-n}[\hat{B}, \hat{B}]. This argument also gives the result on the number of negative eigenvalues of Max4PC_T[B, B]. Hence, by the induction hypothesis, Inertia(Max4PC_T[B, B]) = (0, n - p, n - p).

Since $\operatorname{Max4PC}_T$ is a real symmetric matrix, there exists an orthogonal matrix Q such that $Q\operatorname{Max4PC}_TQ^t = \begin{bmatrix} \operatorname{Max4PC}_T[B, B] & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$. Hence, the result holds by applying Theorem 12. \Box

In our final result, we explicitly describe the eigenvalues of $Max4PC_T$ when T is a star tree.

Theorem 14. Let S_n be the star tree on n vertices. Then, we have

$$\det(xI - \text{Max4PC}_{S_n}) = x^{\binom{n}{2}-2} \left(x^2 - 2(n-1)^2 x - (n-1)\binom{n-1}{2} \right)$$

and the nonzero eigenvalues of $Max4PC_{S_n}$ are

$$(n-1)^2 \pm \sqrt{(n-1)^4 + (n-1)\binom{n-1}{2}}.$$

Proof. Clearly, rank(Max4PC_{S_n}) = 2. Let λ and μ be the two nonzero eigenvalues of Max4PC_{S_n}. Now note that

$$\operatorname{Max4PC}_{S_n} = \begin{bmatrix} 2J_{(n-1)\times(n-1)} & 3J_{(n-1)\times\binom{n-1}{2}} \\ 3J_{\binom{n-1}{2}\times(n-1)} & 4J_{\binom{n-1}{2}\times\binom{n-1}{2}} \end{bmatrix}.$$

Therefore, $\lambda + \mu = 2(n-1) + 4\binom{n-1}{2} = 2(n-1)^2$. Further, note that the sum of all 2×2 principal minors of Max4PC_{*s_n*} is $-(n-1)\binom{n-1}{2}$. It follows that

$$\lambda \mu = -(n-1)\binom{n-1}{2}.$$

Solving the quadratic gives us the two individual roots. Further, the characteristic polynomial of $Max4PC_{S_n}$ is given by

$$x^{\binom{n}{2}-2}\left(x^2-2(n-1)^2x-(n-1)\binom{n-1}{2}\right).$$

This completes the proof. \Box

Declaration of competing interest

There is no competing interest.

Data availability

No data was used for the research described in the article.

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