

On the Inverse and the Dual Index of a Tree

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The inverse of a graph with the spectrum $\lambda_1, \lambda_2, \dots, \lambda_n$ ($\lambda_i \neq 0$) is a graph with the spectrum $1/\lambda_1, 1/\lambda_2, \dots, 1/\lambda_n$. We present a purely graph-theoretic construction of the inverse of a tree with a perfect matching. We apply this method for deriving results concerning the least nonnegative eigenvalue of a tree (called the *dual index* of a tree), including the best possible upper bound for the dual index of a tree in terms of the number of its vertices.

INTRODUCTION

Let \mathbf{G} be a finite undirected graph on n vertices with the spectrum

$$\lambda_n(\mathbf{G}) \leq \lambda_{n-1}(\mathbf{G}) \leq \dots \leq \lambda_2(\mathbf{G}) \leq \lambda_1(\mathbf{G}) = \lambda(\mathbf{G}),$$

where $\lambda_i(\mathbf{G}) \neq 0$ for all i (i.e. the adjacency matrix $A(\mathbf{G})$ of \mathbf{G} is nonsingular). A graph \mathbf{H} will be called an *inverse* of \mathbf{G} iff \mathbf{H} is a graph on n vertices with the spectrum

$$\frac{1}{\lambda_n(\mathbf{G})}, \frac{1}{\lambda_{n-1}(\mathbf{G})}, \dots, \frac{1}{\lambda_2(\mathbf{G})}, \frac{1}{\lambda_1(\mathbf{G})}.$$

Note that there may exist several inverses of \mathbf{G} , in other words the inverse of \mathbf{G} is not determined uniquely. Every graph cospectral with some inverse of \mathbf{G} is an inverse of \mathbf{G} as well. One general way to construct the inverse of a graph \mathbf{G} is to look for a graph \mathbf{H} with the property that $A^{-1}(\mathbf{H})$ —the inverse of its adjacency matrix—is similar to $A(\mathbf{G})$.

The motivation for this research is the fact that the notion of the inverse of a graph can serve as a tool for investigation of properties of the least nonnegative eigenvalue of a graph (a problem of great interest in quantum chemistry). Let us outline the connections between inverses of graphs, inverses of matrices and least nonnegative eigenvalues briefly.

Denote the least nonnegative eigenvalue of \mathbf{G} by $\lambda^+(\mathbf{G})$ and let us call it the *dual index* of \mathbf{G} . There are two possibilities: $\lambda^+(\mathbf{G}) = 0$ or $\lambda^+(\mathbf{G}) \neq 0$. In the first case $A(\mathbf{G})$ is a singular matrix, so no inverse of $A(\mathbf{G})$ exists and the inverse of \mathbf{G} is not defined. In the class of trees this happens iff \mathbf{G} has no perfect matching.

Let \mathbf{G} be a bipartite graph with $A(\mathbf{G})$ nonsingular. Then $A^{-1}(\mathbf{G})$ exists, moreover, if $\det(A(\mathbf{G})) = 1$ then the entries of $A^{-1}(\mathbf{G})$ are natural integers, and if \mathbf{G} is a tree

with perfect matching then $A^{-1}(\mathbf{G})$ is even a $(-1, 0, 1)$ -matrix. It was first observed by Cvetković et al. [4] that if \mathbf{T} is a tree with a perfect matching and $A^+(\mathbf{G})$ is the matrix obtained from $A^{-1}(\mathbf{G})$ by replacing all -1 by $+1$, then $A^{-1}(\mathbf{G})$ is similar to $A^+(\mathbf{G})$ and hence, as long as $A^+(\mathbf{G})$ is a symmetric $(0, 1)$ -matrix, it is the adjacency matrix of some graph, the inverse \mathbf{T}^+ of \mathbf{T} (Cvetković et al. have called the graph pseudoinverse graph). Moreover, Godsil [2] proved that $A^+(\mathbf{G})$ is even diagonally similar to $A^{-1}(\mathbf{G})$. In fact, he proved a more general result:

THEOREM A [2] *Let \mathbf{G} be a bipartite graph on n vertices with unique perfect matching M and let the graph \mathbf{G}/M obtained from \mathbf{G} by contracting edges in M be bipartite as well. Then the following holds:*

- (i) $A^{-1}(\mathbf{G})$ is diagonally similar to the $(0, 1)$ -matrix $A^+(\mathbf{G})$;
- (ii) $\mathbf{G} \subset\subset \mathbf{G}^+$;
- (iii) $\mathbf{G}^+ \subset\subset \mathbf{P}_n^+$.

What can we now say about the dual index of \mathbf{G} ? The key fact is the obvious equality

$$\lambda^+(\mathbf{G}) = \frac{1}{\lambda(\mathbf{G}^+)}. \quad (1)$$

There are some well elaborated methods in spectral graph theory that allow to read information about the index of a graph from its structure. Unfortunately, this is not true for the dual index. However, the equality (1) provides for possibility to use properties of the index of a graph for deriving some properties of the dual index, assuming \mathbf{G}^+ is known. Particularly, Godsil used Theorem A in order to derive the following results, concerning $\lambda^+(\mathbf{G})$:

THEOREM B [2] *Let \mathbf{G} be a bipartite graph on n vertices with unique perfect matching M and let \mathbf{G}/M be bipartite. Then*

- (i) $\lambda(\mathbf{G}) \cdot \lambda^+(\mathbf{G}) \geq 1$ with equality iff $\mathbf{G} \simeq \mathbf{G}^+$;
- (ii) If \mathbf{G} is a forest, then $\lambda^+(\mathbf{G}) \geq \lambda^+(\mathbf{P}_n)$.

In this paper, we will focus our attention on the case of trees with a perfect matching. Let us note that these trees clearly satisfy assumptions of Theorems A and B. In Section 2 we present a purely graph-theoretic construction of the inverse of a tree with a perfect matching. The construction allows us to derive some structural properties of inverses of trees in Section 3. Every theorem proved in this section has consequences for the dual index of a tree, as shown in Section 4.

1. NOTATION

Let us establish some notation and terminology. All graphs in this paper are finite undirected graphs without loops and multiple edges. The edge and the vertex sets of a graph \mathbf{G} are denoted by $E(\mathbf{G})$ and $V(\mathbf{G})$, respectively. We write $\mathbf{G} \subset\subset \mathbf{H}$ if \mathbf{G} is a subgraph of \mathbf{H} and $\mathbf{G} \simeq \mathbf{H}$ if the graphs are isomorphic.

A labeling of a graph G is a mapping $l : E(G) \rightarrow Z$, where Z is the set of all positive integers. As usual, given a labelling l of G with the vertex set $V(G) = \{v_1, \dots, v_n\}$ we define the adjacency matrix $(a_{ij}) = A(G)$ of G to be the square matrix of order n with $a_{ij} = 0$ if $(v_i, v_j) \notin E(G)$ and $a_{ij} = l(v_i, v_j)$ otherwise. Unlabeled graphs may be considered as the labeled graphs with all edges labeled by ones. For a graph G we denote by $\lambda(G)$ and $\lambda^+(G)$ the index of G (that is the greatest eigenvalue of $A(G)$) and the dual index of G (that is the least nonnegative eigenvalue of $A(G)$), respectively.

Our paper deals nearly exclusively with trees. The property of any tree T being bipartite is of great importance in this paper. We say (R, C) is a *bipartition* of G if the sets $R \subset V(G)$ and $S \subset V(G)$ partition $V(G)$ into independent vertex sets and $R \cup S = V(G)$. For given bipartition (R, C) of G it is possible to define an $|R| \times |C|$ matrix $(b_{ij}) = B_{RC}(G)$ by

$$b_{ij} = \begin{cases} l(v_i, v_j) & \text{if } (v_i, v_j) \in E(G), \text{ where } v_i \in R \text{ and } v_j \in C; \\ 0 & \text{otherwise.} \end{cases}$$

This matrix is slightly less familiar than $A(G)$. We will call it the *bipartition matrix* of G corresponding to (R, C) .

It is clear that

$$A(G) = \begin{pmatrix} 0 & B_{RC}(G) \\ B_{RC}^T(G) & 0 \end{pmatrix}.$$

Moreover, if $B_{RC}(G)$ is square nonsingular, then $A(G)$ is nonsingular, too.

Like in the case of adjacency matrix, the matrix $B_{RC}(G)$ depends essentially on the assignment of vertices of the graph to the rows and columns of the matrix. A perfect matching in a graph G will be denoted by $M(G)$, $M(G) \subset E(G)$. We say that the bipartition matrix $B_{RC}(G)$ matches the perfect matching $M(G)$ if the edges in $M(G)$ correspond to the diagonal entries of $B_{RC}(G)$, in other words the vertices in $R = \{r_1, \dots, r_{n/2}\}$ and $C = \{s_1, \dots, s_{n/2}\}$ are ordered so that $(r_i, s_j) \in M(G)$ iff $i = j$.

A path on n vertices will be denoted by P_n . A path in G of length k is a subgraph of G isomorphic to P_{k+1} . Given a perfect matching $M(G)$ in a graph G we say that a path P in G is *alternating* if in every pair of incident edges in P there is exactly one edge that belongs to $M(G)$. An alternating path is said to be *poor* if it is of length at least three and if it contains more edges that do not belong to $M(G)$ than the ones that belong to $M(G)$. It is clear that every poor alternating path has an even number of vertices.

A *pending path* P in G is a path in G such that all vertices of P are of degree two in G except the end vertices of P ; one endvertex is of degree one and the second one of degree at least two in G —this vertex is called a *vertex of attachment* of P to G ; denote it by v . A pending path of length one is simply a *pending edge*. If the degree of v in G is at least three, then P is called the *maximal* pending path. It will be also said that G is obtained by *gluing* an endvertex of P to the vertex of attachment v .

Finally, for $V \subset V(G)$ we denote by $G \setminus V$ the graph induced by G by $V(G) \setminus V$ and for $E \subset E(G)$ we denote by $G \setminus E$ the graph obtained from G by deleting the edges

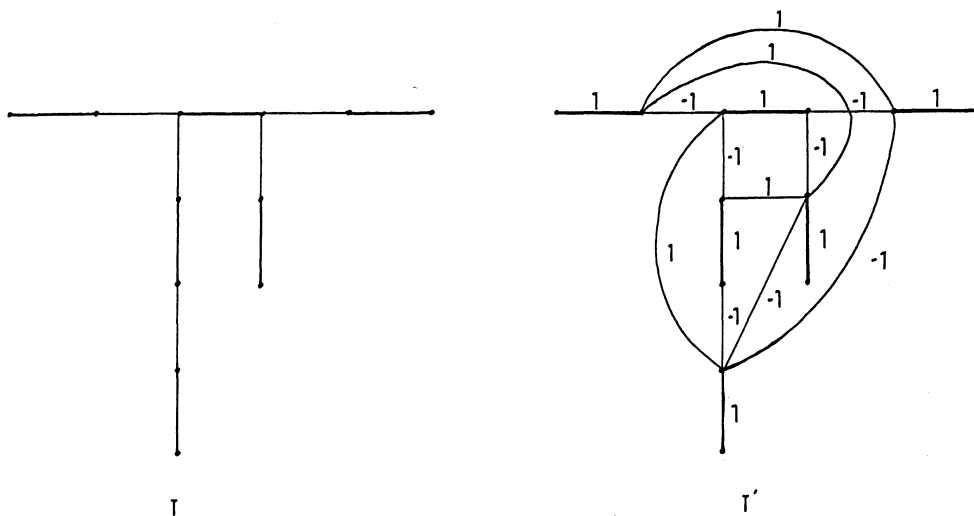


FIGURE 1.

in E . For $v \in V(\mathbf{G})$ and $e \in E(\mathbf{G})$ we will write $\mathbf{G} \setminus v$ and $\mathbf{G} \setminus e$ instead of $\mathbf{G} \setminus \{v\}$ and $\mathbf{G} \setminus \{e\}$, respectively.

2. CONSTRUCTION AND SIMPLE PROPERTIES OF \mathbf{T}^+

Let \mathbf{T} be a tree with a perfect matching M . Our goal is to provide a construction of a graph \mathbf{T}' , the adjacency matrix of which is the matrix $A^{-1}(\mathbf{T})$. Because $A^{-1}(\mathbf{T})$ is a $(0, 1, -1)$ matrix, the edges of \mathbf{T}' have to be labeled by numbers $+1$ or -1 . The construction is as follows:

\mathbf{T}' has the same vertex set as \mathbf{T} and its edge set is a superset of the edge set of \mathbf{T} . First, let us label the edges of \mathbf{T} in the following simple way: If an edge e is in the perfect matching $M(\mathbf{G})$, put $l(e) = +1$; otherwise put $l(e) = -1$. Now, add new labelled edges to \mathbf{T} : we join two vertices u, v in \mathbf{T} by a new edge e iff there exists a poor alternating path in \mathbf{T} that joins vertices u and v . If the distance between v and u along the alternating path is $3 \pmod 4$, then $l(e) = +1$; if it is $1 \pmod 4$, then $l(e) = -1$. Figure 1 illustrates a simple tree \mathbf{T} and constructed \mathbf{T}' .

Note that \mathbf{T} being a tree implies that the alternating path is unique, and hence the definition of \mathbf{T}' is correct.

THEOREM 1 *Let \mathbf{T} be a tree with a perfect matching. Then the adjacency matrix of the graph \mathbf{T}' constructed above is the inverse of the adjacency matrix of \mathbf{T} : $A(\mathbf{T}') = A^{-1}(\mathbf{T})$.*

Proof It can be easily seen from the construction that \mathbf{T}' contains no cycles of odd length and hence \mathbf{T}' is bipartite. Since \mathbf{T}' is a subgraph of the connected bipartite graph \mathbf{T} with bipartition (R, C) , (R, C) is also a bipartition of the vertex set of \mathbf{T}' . Hence we may construct some bipartition matrix $B_{RC}(\mathbf{T}')$; let us choose the one that matches $M(\mathbf{T}) = M(\mathbf{T}') = M$. Let $B_{RC}(\mathbf{T})$ be a bipartition matrix of

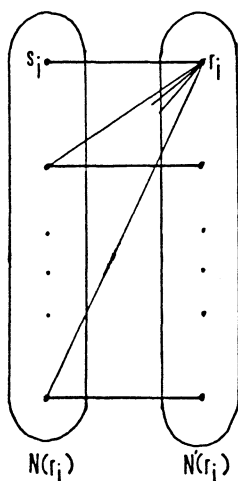


FIGURE 2.

T that matches M , too. Then it suffices to prove that $B_{RC}(T') = B_{RC}^{-1}(T)$. Define $D = (d_{ij}) = B_{RC}(T) \cdot B_{RC}(T')$. We shall prove that $D = I$.

Take an arbitrary fixed pair r_i, s_j of vertices in T' such that $r_i \in R$ and $s_j \in C$. Denote the neighborhood of r_i in T by $N(r_i)$ and define $N'(r_i) = \{u \in V(T) \mid (v, u) \in M \text{ and } v \in N(r_i)\}$. $N'(r_i)$ contains vertices “matched” with vertices in $N(r_i)$ by the perfect matching M (see Fig. 2). Note that $r_i \in N'(r_i)$.

Now, a graph-theoretic formulation of the matrix multiplication tells us that the ij entry of D equals to

$$d_{ij} = \sum_{e \in E_{ij}} l(e),$$

where $E_{ij} = \{(u, s_j) \in E(T') \mid u \in N'(r_i)\}$ is the set of all edges in T' that join s_j with some vertex in $N'(r_i)$.

Let us consider 3 cases:

- (i) Case $(r_i, s_j) \in M$. Because the matrices $B_{RC}(T)$ and $B_{RC}(T')$ match M this is equivalent to $i = j$. Suppose there is an edge in E_{ij} , different from (r_i, s_j) , say (r, s_j) is in E_{ij} . But then $r \in N'(r_i)$ and hence there is a cycle $s_j r_i s r$ in T —a contradiction (see Fig. 3a).
Hence $E_{ij} = \{(r_i, s_j)\}$ and by the definition of the labeling l of T' , $d_{ij} = d_{ii} = 1$ for all i .
- (ii) Case $s_j \in N(r_i)$, but $i \neq j$. There is only one path connecting s_j and any $r \in N'(r_i)$, $r_j \neq r \neq r_i$ in T —the path $r s r_i s_j$ (see Fig. 3b). This path is not alternating, and hence there is not an edge (s, r_j) in T' . Hence E_{ij} contains only two edges, namely (r_j, s_j) and (r_i, s_j) . By the definitions of the labeling l we have that $l(r_j, s_j) = 1$ and $l(r_i, s_j) = -1$, and hence $d_{ij} = 0$.
- (iii) Case $s_j \notin N(r_i)$ (Fig. 4). If $E_{ij} = \emptyset$ then trivially $d_{ij} = 0$. Suppose now that $E_{ij} \neq \emptyset$ and let $(r_k, s_j) \in E_{ij}$. Then $k = i$ or $k \neq i$ and $(r_k, s_j) \in E(T)$ or

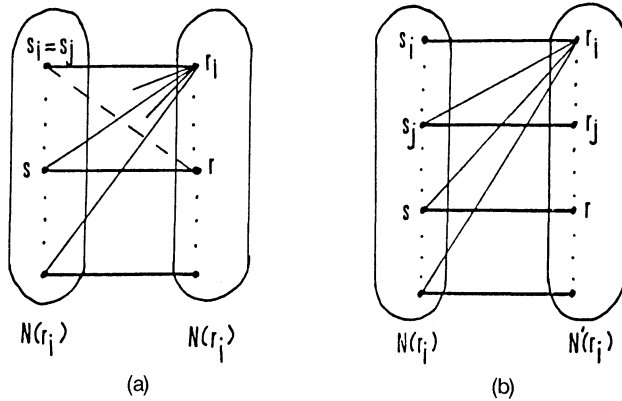


FIGURE 3.

$(r_k, s_j) \notin E(\mathbf{T})$, which yields to four subcases. One of them is a contradiction: if $i = k$ then $(s_j, r_i) \in E(\mathbf{T})$ implies $s_j \in N(r_i)$ —a contradiction. The remaining three subcases are meaningful:

- (a) Subcase $i = k$ and $(s_j, r_i) \notin E(\mathbf{T})$. Then by the construction of \mathbf{T} there is a poor alternating path \mathbf{P} that joins $r_i = r_k$ and s_j . The vertex that is adjacent to r_k in \mathbf{P} belongs to $N(r_i)$; say it is the vertex s_t (Fig. 4). Define $\bar{\mathbf{P}} = \mathbf{P} \setminus \{r_i, s_t\}$. If the length of $\bar{\mathbf{P}}$ equals 1, then $(r_t, s_j) \in E_{ij}$, moreover $(r_t, s_j) \in E(\mathbf{T}) \setminus M$ and hence $l(r_t, s_j) = -1$; consequently the length of the path \mathbf{P} equals 3 and hence $l(r_i, s_j) = 1 = -l(r_t, s_j)$. If the length of $\bar{\mathbf{P}}$ is greater than 1 then $\bar{\mathbf{P}}$ is a poor alternating path joining s_j and r_t and hence $(r_t, s_j) \in E(\mathbf{T}')$. It is clear that $(r_t, s_j) \in E_{ij}$ and $l(r_t, s_j) = -l(r_i, s_j)$.
- (b) Subcase $i \neq k$ and $(s_j, r_k) \in E(\mathbf{T})$. Then clearly $(s_j, r_k) \notin M$ and moreover $s_j r_k s_k r_i$ is a poor alternating path of length 3, and hence $(r_i, s_j) \in E_{ij}$, $l(r_i, s_j) = 1 = -l(r_k, s_j)$.
- (c) Subcase $i \neq k$ and $(s_j, r_k) \notin E(\mathbf{T})$. Then there is a poor alternating \mathbf{P} in \mathbf{T} joining s_j and r_k . \mathbf{P} in conjunction with the edges (r_k, s_k) and (s_k, r_i) form another alternating path $\bar{\mathbf{P}}$ in \mathbf{T} joining r_i and s_j , and hence $(r_i, s_j) \in E_{ij}$. It is clear that $l(r_i, s_j) = -l(r_k, s_j)$.

As we have seen, in all subcases if E_{ij} is nonvoid then it contains at least two edges e_1 and e_2 such that $l(e_1) = -l(e_2)$. Suppose for a moment that there is another edge e_3 in E_{ij} . It means that there is another path \mathbf{Q} in \mathbf{T} connecting s_j with some vertex in $N'(r_i)$, say r . But then there is also a path $\bar{\mathbf{Q}}$ in \mathbf{T} that connects s_j and r_i ; the path $\bar{\mathbf{Q}}$ contains the vertex r . The path \mathbf{P} (or $\bar{\mathbf{P}}$) from s_j to r_i found above does not contain r ; indeed otherwise there is a cycle in \mathbf{T} —a contradiction. But then there are two distinct paths connecting s_j and r_i in \mathbf{T} —a contradiction with \mathbf{T} being a tree.

Finally, we can conclude that if $E_{ij} = \emptyset$ then there are exactly two edges e_1, e_2 in E_{ij} such that $d_{ij} = l(e_1) + l(e_2) = 0$.

The proof of the theorem is complete. ■

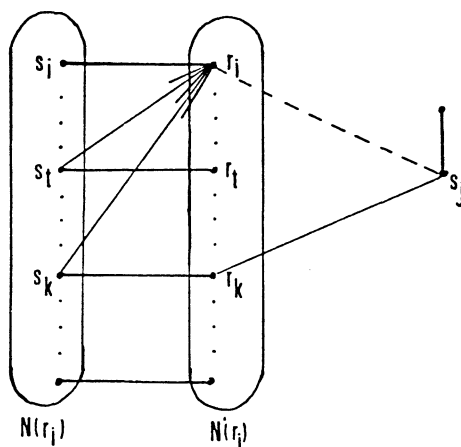


FIGURE 4.

COROLLARY 1 *The inverse T^+ of a tree T with a perfect matching is obtained by adding new edges to T according to the following rule: $(u, v) \in E(T^+) \setminus E(T)$ iff there is a poor alternating path joining u and v in T .*

Proof Let T' be the graph from Theorem 1. Then according to this theorem $A^{-1}(T) = A(T')$; moreover Theorem A implies that $A(T')$ is similar to $A(T^+)$. ■

Let us now list some simple, but interesting and powerful properties of T^+ .

Note 1

- (a) $T \subset\subset T^+$ by the construction;
- (b) Since an endvertex of T can not be an endvertex of any poor alternating path, the set of all endvertices of T^+ equals to those of T .

Note 2 It is easily checked that T^+ is a bipartite graph with unique perfect matching, and hence $M(T) = M(T^+)$ is the unique perfect matching in T^+ . Moreover, the bipartition (R, C) of T is the bipartition of T^+ too.

Note 3 Let $F \subset\subset T$ be a forest with a perfect matching such that $M(F) \subset M(T)$. Then clearly each poor alternating path in F is a poor alternating path in T , and hence $F^+ \subset\subset T^+$.

Note 4 Gudsil [2] has proved that if T has n vertices then $T^+ \subset\subset P_n^+$ (see Theorem A, (iii)). By Note 2 the inverse of P_n is a bipartite graph with unique perfect matching and it is easy to verify using Corollary 1 that P_n^+ has exactly $m(m+1)/2$ edges, where $n = 2m$. It is interesting that in general if G is a bipartite graph with unique perfect matching on $2m$ vertices then $|E(G)| \leq m(m+1)$; this follows immediately e.g. from [2], Lemma 2.1. Hence P_n^+ is the extremal graph with respect to this property.

Note 5 Due to Theorem B, (i) $\lambda^+(T) = 1/\lambda(T)$ iff $T \simeq T^+$. Graphs with this property are called *self-inverse graphs*. Self-inverse trees have been characterized

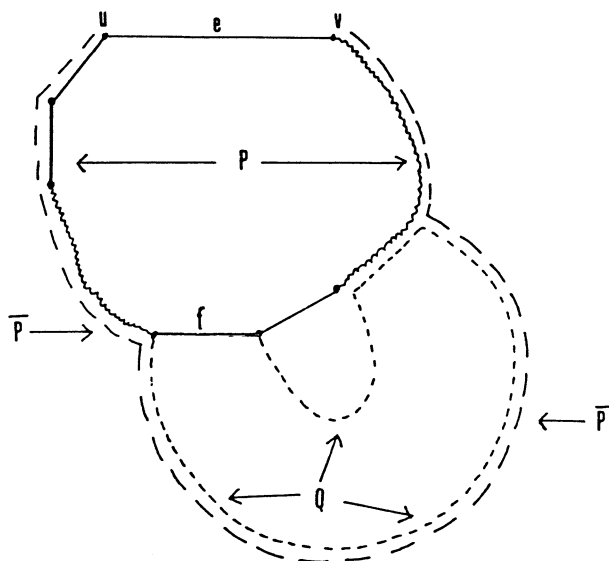


FIGURE 5.

by Godsil: A tree T on $2m$ vertices with a perfect matching is self-inverse iff it can be constructed from a tree \bar{T} on m vertices by gluing P_2 to each vertex in \bar{T} . Note that this characterization is easily obtained from Corollary 1.

Note 6 The construction of T^+ can be reformulated in the following way (which is more suitable for routine derivation of T^+ from T): For all pairs of distinct end-vertices in T construct the inverses of the (uniquely determined) alternating paths joining these pairs in T . If in the resulting graph there are multiple edges, take only one of them. The graph that results is T^+ (cf. Fig. 1).

Note 3 allows the following remarkable generalization:

THEOREM 2 *Let T be a tree with a unique perfect matching and let F be a subforest of T^+ with a perfect matching such that $M(F) \subset M(T^+) = M(T)$. Then $F^+ \subset\subset T^+$.*

Proof Let e be an edge in F^+ . If $e \in E(F)$, then by the assumption also $e \in E(T^+)$. On the other hand, if $e = (u, v) \notin E(F)$ then due to Corollary 1 there is an alternating path P in F that joins vertices u and v . If all edges of P belong to $E(T)$ then (because of $M(F) \subset M(T)$) P is also a poor alternating path in T , and hence—again by Corollary 1— $e \in E(T^+)$.

Now, let there be k edges in P that do not belong to T ; take one of them, say f . But as $f \in E(T^+)$ then by Corollary 1 there is a poor alternating path Q in T that connects the endvertices of f . We can combine parts of $P \setminus f$ and Q in such a way that we obtain a poor alternating path \bar{P} connecting u and v which contains at most $k - 1$ edges that do not belong to T (see Fig. 5). By repeated use of this procedure we obtain a poor alternating path \bar{P} in T , joining u and v , yielding $(u, v) \in E(T^+)$. ■

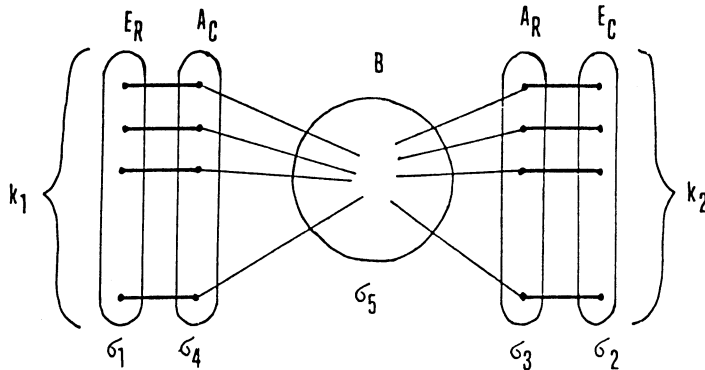


FIGURE 6.

3. FURTHER PROPERTIES OF T^+

We start with a kind of extremal problem related to the inverses of trees:

THEOREM 3 *Let T be a tree on $2m$ vertices with a perfect matching and bipartition (R, C) . Let the number of endvertices of T that belong to the partition set R (resp. C) equal k_1 (resp. k_2). Then for $k_1 + k_2 < m$ the number of edges in the inverse graph T^+ of T is*

$$|E(T^+)| \leq e = \frac{1}{2}(m(m + 1) - k_1(k_1 - 1) - k_2(k_2 - 1)), \tag{2}$$

and this is the best bound.

Proof According to Notes 1 and 2, T^+ is a bipartite supergraph of T with the bipartition (R, C) , and the endvertices in T^+ are exactly the endvertices in T .

Consider the following set of vertices in T^+ : E_R —the set of endvertices in partition R , A_C —the set of vertices in C , adjacent to vertices in E_R , E_C —the set of endvertices in partition C , A_R —the set of vertices in R , adjacent to vertices in E_C , and finally B —the set of remaining vertices (see Fig. 6).

It is clear that

$$\begin{aligned} |E_R| &= |A_C| = k_1; \\ |E_C| &= |A_R| = k_2; \\ |B| &= 2m - 2k_1 - 2k_2. \end{aligned}$$

Denote by $\sigma_1, \sigma_2, \sigma_3, \sigma_4$ and σ_5 the sums of degrees of vertices in the sets E_R, E_C, A_R, A_C and B , respectively. Then $\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4 + \sigma_5$ is equal to the sum of degrees of all vertices in T^+ , hence $2|E(T^+)|$.

By the definition, $\sigma_1 = k_1, \sigma_2 = k_2$.

Next, let v be a vertex in A_R adjacent to $u \in E_C$. The vertex v is surely adjacent neither to any vertex that belongs to R , nor to any vertex from E_C , except of u . Hence

$$\delta(v) \leq m - k_2 + 1 \quad \text{and therefore} \quad \sigma_3 \leq k_2(m - k_2 + 1).$$

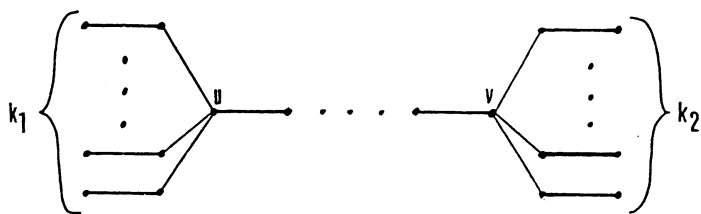


FIGURE 7.

Similarly,

$$\sigma_4 \leq k_1(m - k_1 + 1).$$

Finally, let us consider B . Since \mathbf{T}^+ is a bipartite graph with unique 1—factor, the subgraph \mathbf{F} of \mathbf{T}^+ induced by B is bipartite with unique 1—factor itself, and hence (see Note 4)

$$\begin{aligned} 2|E(\mathbf{F})| &\leq \frac{1}{2}|\mathcal{V}(\mathbf{F})| \cdot (\frac{1}{2}|\mathcal{V}(\mathbf{F})| + 1) \\ &= (m - k_1 - k_2) \cdot (m - k_1 - k_2 + 1). \end{aligned}$$

Every vertex in B that belongs to R (resp. C) could additionally be connected to any vertex in \mathcal{A}_C (resp. \mathcal{A}_R) in graph \mathbf{T}^+ . This implies that

$$\begin{aligned} \sigma_5 &\leq (m - k_1 - k_2) \cdot (m - k_1 - k_2 + 1) + (k_1 + k_2) \cdot (m - k_1 - k_2) \\ &= (m + 1) \cdot (m - k_1 - k_2). \end{aligned}$$

Summarizing these partial results we obtain that

$$\begin{aligned} 2|E(\mathbf{T}^+)| &= \sigma_1 + \sigma_2 + \sigma_3 + \sigma_4 + \sigma_5 \\ &\leq k_1 + k_2 + k_1(m - k_1 + 1) + k_2(m - k_2 + 1) \\ &\quad + (m + 1) \cdot (m - k_1 - k_2) \\ &= k_1 - k_1^2 + k_2 - k_2^2 + (m + 1) \cdot (k_1 + k_2) + (m + 1)m \\ &\quad - (m + 1) \cdot (k_1 + k_2) \\ &= m(m + 1) - k_1(k_1 + 1) - k_2(k_2 + 1), \end{aligned}$$

which proves the bound (2). To prove that the bound is the best possible it is enough to consider the graph in Fig. 7. The length l of the path joining vertices u and v in the figure equals $l = 2m - 2k_1 - 2k_2$, yielding $l > 0$ because of the assumption $k_1 + k_2 > m$.

It is not difficult to verify that the number of edges of the inverse of \mathbf{T} equals to the upper bound in (2).

The proof is complete. ■

Let us note that if $k_1 + k_2 = m$ then the construction of the graph in Fig. 7 is not applicable. However, due to Note 5 this is the case of self-inverse graphs, and hence in this case $|E(\mathbf{T}^+)| = |E(\mathbf{T})| = 2m - 1$. Moreover, it is clear that there is no

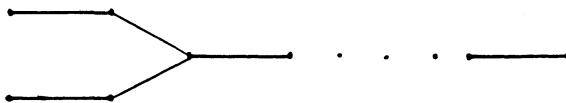


FIGURE 8.

invertible graph with $k_1 + k_2 > m$ endvertices, and hence Theorem 3 and Note 5 cover all interesting cases.

Owing to Note 1, T is a spanning tree in T^+ . We are going to show that in every T^+ there is another interesting spanning tree. Let us prove first the following lemma:

LEMMA 1 *Let T be a tree on $2m$ vertices with a perfect matching. Denote by S the set of all vertices of T^+ adjacent to its endvertices. Then the subgraph of T^+ induced by S is connected in $T^+ \setminus M(T^+)$.*

Proof We shall proceed by induction on m . For $m = 1$ the lemma is trivial. If $m > 1$ take an endvertex v of T and the vertex u adjacent to v . The components T_1, \dots, T_k of $T \setminus \{u, v\}$ are trees with a perfect matching; denote by S_i the set of all vertices in T_i that are adjacent to its endvertices. Because T has a perfect matching, there is at least one vertex $s_i \in S_i$ such that there is an alternating path in T^+ joining u and s_i for every i , and hence by Corollary 1 $(u, s_i) \in E(T^+)$; moreover $(u, s_i) \notin M(T^+)$. On the other hand, $T_i^+ \subset T$ for all i due to Note 3, and so—by the induction— S_i induces a connected subgraph in $T^+ \setminus M(T^+)$. Hence $S = \bigcup_{i=1, \dots, k} S_i \cup \{u\}$ induces a connected subgraph of T^+ . ■

THEOREM 4 *Let T be a tree with a perfect matching M . Then T^+ contains a self-inverse spanning tree.*

Proof The perfect matching $M = M(T)$ groups the vertices in T into pairs. This set of all pairs can be divided into two disjoint sets: the set A that contains pairs of vertices exactly one of which is an endvertex of T and the set B containing pairs of vertices none of which is an endvertex. Now, take from each pair in A a vertex that is not an endvertex; the set S formed in this way induces a subgraph in $T^+ \setminus M$ that is connected by Lemma 1. Now, choose any vertex v from any pair in B .

Since T is a tree with a perfect matching it is easily seen that there are at least two vertices u_1, u_2 in S joined with v by alternating paths. Moreover, one of the paths is poor; say the path to u_1 is poor. Hence by Corollary 1 there is an edge (v, u_1) in T^+ that does not belong to M . Consequently, there is a connected subgraph H in $T^+ \setminus M$ that contains exactly one vertex from each pair in $A \cup B$. Let \bar{H} be any spanning tree in H and let G be the graph obtained from \bar{H} by joining the vertices of \bar{H} with the remaining vertices in pairs from $A \cup B$ by corresponding edges from M . Then G is a self-inverse spanning tree in T^+ . ■

According to Note 4 every T^+ is a subgraph of the inverse of the path on the same number of vertices n . Now, we are going to prove a little stronger result, namely that if T is not a path then T^+ is a subgraph of Z_n^+ , where Z_n is the graph on n vertices shown in Fig. 8.

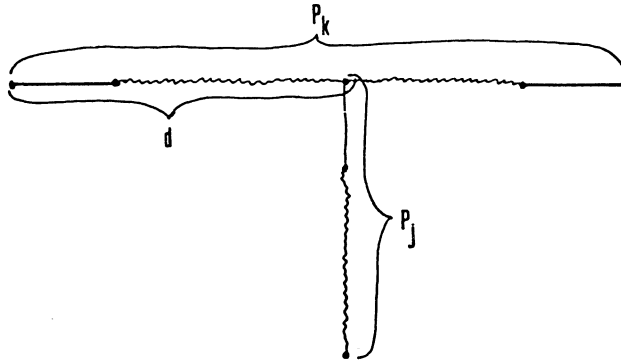


FIGURE 9.

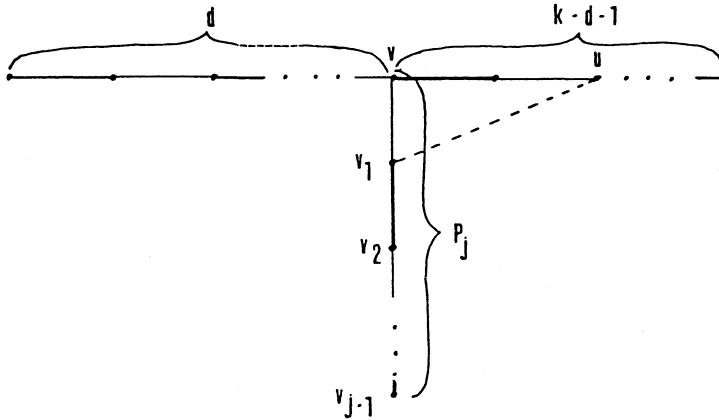


FIGURE 10.

First, let us prove the claim in the special case of trees with exactly 3 endvertices.

Every graph with a perfect matching that has 3 endvertices can be constructed by gluing an endvertex of a path P_j to some vertex (but not an endvertex) of a path P_k ; let us choose some endvertex in P_k and denote by d the distance between the chosen endvertex and the vertex of attachment of P_j to P_k (see Fig. 9).

Denote the graph described above by $T_{k,j,d}$. It is clear that $T_{k,j,0} \simeq T_{k,j,k-1} \simeq P_{k+j-1}$.

LEMMA 2 *Let $T_{k,j,d}$ have a perfect matching and let P_k be an alternating path in $T_{k,j,d}$. Then*

- (a) $T_{k,j,d}^+ \supset \supset T_{k,j,d+2}^+$ for all d even, $d < k - 3$;
- (b) $T_{k,j,d}^+ \subset \subset T_{k,j,d+2}^+$ for all d odd, $d < k - 1$.

Proof Let $d < k - 3$ be even and denote by u the vertex in P_k whose distance from the chosen endvertex of P_k equals $d + 2$ (Fig. 10).

By the use of Corollary 1 it can be easily seen that $E(T_{k,j,d}^+) = E(T_{k,j,d+2}^+) \cup \{(u,v), (u,v_3), (u,v_5), \dots, (u,v_{j-1})\}$. The case of d odd is symmetric to the previous

one, because $T_{k,j,d}$ is isomorphic to $T_{k,j,k-d-1}$ and k is even (as P_k is the alternating path in $T_{k,j,d}$), so $k - d - 1$ is even if d is odd. ■

LEMMA 3 *Let T be a tree on n vertices with a perfect matching. Let T have exactly 3 endvertices. Then $T^+ \subset\subset Z_n^+$.*

Proof T is isomorphic to a $T_{k,j,d}$ for some k, j and d , where P_k is an alternating path in $T_{k,j,d}$, d is even, $0 < d < k - 1$ and j is odd. If $d < k - 1$ then $T_{k,j,d}^+ \subset\subset T_{k,j,2}^+$ by the repeated use of Lemma 2a). Now, $T_{k,j,2} \simeq T_{k+j-3,3,j-1}$, where P_{k+j-3} is an alternating path in $T_{k+j-3,3,j-1}$. Since $j - 1$ is even, again by the repeated use of Lemma 2a) we have $P_{k+j-3,3,j-1}^+ \subset\subset P_{k+j-3,3,2}^+ \simeq Z_n^+$. ■

The following lemma concerning the structure of trees with perfect matching allows us to generalize Lemma 3:

LEMMA 4 *Let T be a tree with a perfect matching, not isomorphic to P_n . Then there is a maximal pending path in T of even length $r, r > 0$.*

Proof Let us first prove that in T there is a pending path of length at least two.

Let k be the number of endvertices in T . The vertices adjacent to these endvertices are pairwise distinct (because T has a perfect matching) and if there is no pending path of length at least two in T , then the degree of every vertex adjacent to an endvertex is at least 3. Hence there are k vertices of degree 1, k vertices of degree at least 3 and $n - 2k$ vertices of degree at least 2 in T . Hence

$$\sum_{v \in V(T)} d(v) \geq 4k + 2(n - 2k) = 2n,$$

a contradiction with T being a tree.

Now, we prove the lemma by induction on n . The smallest n for which a tree with a perfect matching nonisomorphic to the path exists is $n = 6$ and the tree is unique; it is $T_{4,3,1}$. Let $n > 6$ and take some maximal pending path in T of length $r \geq 2$. If r is even then we are done. If r is odd, delete last two vertices of the path from T in order to obtain a tree \bar{T} . \bar{T} has less vertices than T , and hence—by the induction hypothesis—there is a maximal pending path \bar{P} in \bar{T} of even length $\bar{r} > 0$. But the path \bar{P} is also a maximal pending path of even length in T . ■

THEOREM 5 *Let T be a tree on n vertices with a perfect matching. If T is not isomorphic to P_n , then $T \subset\subset Z_n^+$.*

Proof By Lemma 4, there is a maximal pending path P_j of even length $j - 1$ in T ; denote by v the vertex of attachment of this path to T . By the definition of maximal pending path, $\delta_T(v) \geq 3$. Define $\bar{T} = T \setminus (P_j \setminus v)$. By Note 4 $\bar{T}^+ \subset\subset P_k^+$, where $k = |V(\bar{T})|$. Moreover, $\bar{T} \subset\subset \bar{T}^+ \subset\subset P_k^+$, and hence v can be viewed as a vertex in \bar{T}^+ as well as a vertex in P_k^+ . Because v is a vertex in three graphs, by gluing an endvertex of P_j to v we obtain three graphs: the original T (from \bar{T}) and two new graphs: H (from \bar{T}^+) and F (from P_k^+). It is trivial that $T \subset\subset H \subset\subset F$. Due to the construction of F it contains P_k as well as the vertex v to which an endvertex of P_j is glued—in other words, F contains $T_{k,j,d}$ for some d . It is clear that $F \subset\subset T_{k,j,d}^+$.

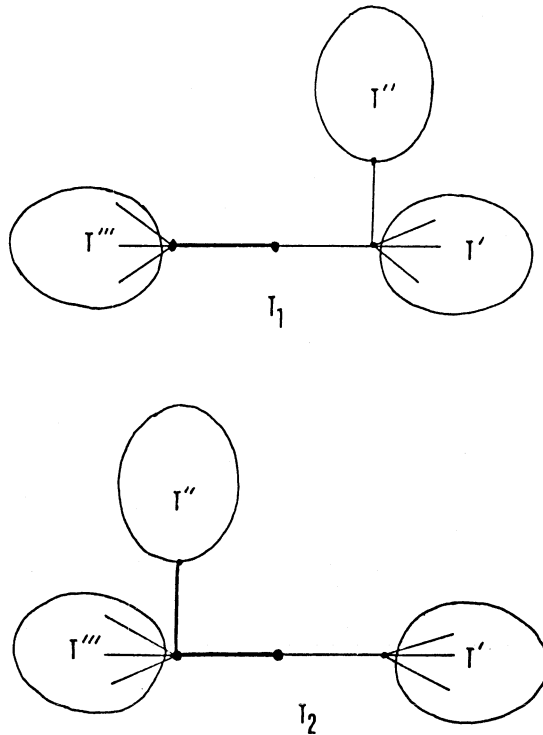


FIGURE 11.

Because $\delta_{T^+}(v) \geq 2$, v is not an endvertex of P_k^+ implying it is not an endvertex of P_k as well and thus yielding $0 < d < k - 1$. Hence $T_{k,j,d}^+ \subset\subset Z_n^+$ by Lemma 3. The chain of inclusions is complete: $T \subset\subset H \subset\subset F \subset\subset T_{k,j,d}^+ \subset\subset Z_n^+$. So $T \subset\subset T_{k,j,d}^+$ and finally by Theorem 3 $T^+ \subset\subset Z_n^+$. ■

Let us note that by the simple method used in the proof of Lemma 1 a number of pairs of trees can be compared with respect to their dual index. For example, if T_1 and T_2 are trees with a perfect matching shown in Fig. 11, then $T_1^+ \subset\subset T_2^+$.

We have proved several theorems concerning structural properties of inverses of trees. Now we are going to show consequences for the dual index.

4. PROPERTIES OF THE DUAL INDEX

Theorems 3–5 have direct consequences concerning the dual index. Let us begin by consequences of Theorem 3. The theorem gives the upper bound on the number of edges in T^+ . There are many results in matrix theory that derive an upper bound for the Perron root of a nonnegative matrix in terms of the sum of its entries.

The following is a graph-theoretic reformulation of a theorem due to Friedland [1]. Note that for every integer e there exists a unique integer k and unique L even such that $e = k(k - 1) + L$ and $0 \leq L < 2k$.

THEOREM C (Friedland [1]) *Let G be a graph on e vertices, let $e = k(k - 1) + L$, where $0 \leq L < 2k$. Then*

$$\lambda(G) \leq \frac{k - 1 + \sqrt{(k - 1)^2 + 2L}}{2}$$

Proof [1], Theorem 9. ■

Now, Theorem 3 together with Theorem C gives the following result:

THEOREM 6 *Let T be a tree with a perfect matching on $2m$ vertices with k_1 endvertices in partition R and k_2 endvertices in partition C . Let*

$$e = \frac{1}{2}(m(m + 1) - k_1(k_1 - 1) - k_2(k_2 - 1)); \tag{3}$$

and let $e = k(k + 1) + L$, $0 \leq L < 2k$. Then

$$\frac{2}{k - 1 + \sqrt{(k - 1)^2 + 2L}} \leq \lambda^+(T).$$

Proof Denote $I = k - 1 + \sqrt{(k^2 - 1) + 2L}$. By Theorem 3 $|E(T^+)| \leq e$ and hence by Theorem C $\lambda(T^+) \leq I/2$. Because $\lambda^+(T) = 1/\lambda(T^+)$, this implies $\lambda^+(T) \geq 2/I$. ■

Now, define $\sigma_n = \max \lambda^+(T)$, where the maximum is taken over the set of all self-inverse trees on n vertices. It follows from Theorem 4 that if T is any tree on n vertices then

$$\lambda^+(T) \leq \sigma_n.$$

As for self-inverse trees $\lambda^+(T) = 1/\lambda(T)$, the problem of determining σ_n is equivalent to the problem of determining $\min \lambda(T)$ over the set of all self-inverse trees on n vertices. The corresponding problem over the set of all trees on n vertices has been solved long ago independently by several authors, including Lovász and Pelikán [3]. The method they used is suitable for solving our problem, too.

LEMMA 5 *Denote by \bar{S}_n and \bar{P}_n the self-inverse graphs on n vertices shown on Fig. 12. If \bar{T} is any self-inverse tree on n vertices then*

$$\lambda(\bar{P}_n) \leq \lambda(\bar{T}) \leq \lambda(\bar{S}_n).$$

Proof Let us first recall a definition and some basic lemmas from the paper [3].

Denote by $f_G(\lambda)$ the characteristic polynomial of a graph G . Let T_1 and T_2 be trees. Let us denote $T_1 < T_2$ if $f_{T_1}(\lambda) \geq f_{T_2}(\lambda)$ for every $\lambda \geq \lambda(T_2)$. The following are the basic properties of $<$:

- (i) $T_1 < T_2$ implies $\lambda(T_1) \leq \lambda(T_2)$;
- (ii) $T_1 \subseteq T_2$ implies $T_1 < T_2$;
- (iii) Let $e = (u_1, v_2)$ and $e' = (u_2, v_2)$ be vertices in T_1 and T_2 , respectively. Then

$$(T_2 \setminus (u_2, v_2)) < (T_1 \setminus (u_1, v_1))$$

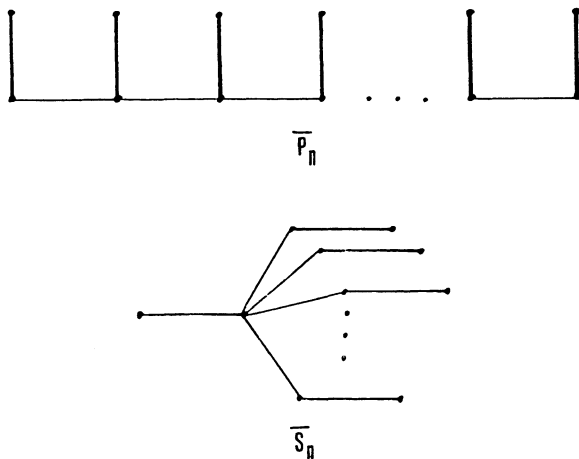


FIGURE 12.

and

$$(\mathbf{T}_1 \setminus \{\mathbf{u}_1, \mathbf{v}_1\}) > (\mathbf{T}_2 \setminus \{\mathbf{u}_2, \mathbf{v}_2\})$$

implies

$$\mathbf{T}_2 < \mathbf{T}_1$$

(cf. [3], Lemmas 2 and 3).

Let $\bar{\mathbf{T}}$ be any self-inverse tree on $n = 2m$ vertices and let \mathbf{T} be the underlying tree on m vertices obtained by deleting endvertices from $\bar{\mathbf{T}}$. Let us prove first that $\bar{\mathbf{P}}_n < \bar{\mathbf{T}}$.

We have to prove that if $\bar{\mathbf{T}}$ is a self-inverse tree on n vertices such that there is no other self-inverse tree $\bar{\mathbf{T}}^*$ on the same number of vertices with $\bar{\mathbf{T}}^* < \bar{\mathbf{T}}$, then $\bar{\mathbf{T}} = \bar{\mathbf{P}}_n$. Assume that there exist vertices of valency at least 3 in underlying \mathbf{T} . Let \mathbf{u} be a vertex in \mathbf{T} such that $\delta_{\mathbf{T}}(\mathbf{u}) \geq 3$ and at least one component of $\mathbf{T} \setminus \mathbf{u}$ is a path. Denote by \mathbf{v}_1 and \mathbf{v}_2 endvertices of this path, \mathbf{v}_1 being adjacent to \mathbf{u} in \mathbf{T} . Let (\mathbf{w}, \mathbf{u}) be another edge incident with \mathbf{u} and put $\mathbf{T}^* = (\mathbf{T} \setminus (\mathbf{w}, \mathbf{u}_2)) \cup (\mathbf{w}, \mathbf{v}_2)$ (see Fig. 13). It is easy to see that $\bar{\mathbf{T}}^*$ is a selfinverse tree, moreover, \mathbf{T}^* has more endvertices than \mathbf{T} , hence $\bar{\mathbf{T}}^* \neq \bar{\mathbf{T}}$. Furthermore, $\bar{\mathbf{T}} \setminus (\mathbf{w}, \mathbf{u}) \simeq \bar{\mathbf{T}}^* \setminus (\mathbf{w}, \mathbf{u}_2)$ and $\bar{\mathbf{T}} \setminus \{\mathbf{u}, \mathbf{v}\}$ is isomorphic to a subgraph of $\bar{\mathbf{T}}^* \setminus \{\mathbf{u}, \mathbf{v}_2\}$. Hence by (i) and (ii) we have $\bar{\mathbf{T}}^* < \bar{\mathbf{T}}$, a contradiction.

Now, let us prove $\bar{\mathbf{T}} < \bar{\mathbf{S}}_n$ by the use of induction on n . The first interesting case is $n = 8$; in this case there are exactly two non-isomorphic self-inverse trees, namely $\bar{\mathbf{P}}_8$ and $\bar{\mathbf{S}}_8$ with $\bar{\mathbf{P}}_8 < \bar{\mathbf{S}}_8$ as proved above. Now, let $n \geq 10$. Let \mathbf{u} be an endvertex of the underlying \mathbf{T} and let (\mathbf{w}, \mathbf{u}) be an edge in \mathbf{T} . Then $\bar{\mathbf{T}} \setminus (\mathbf{w}, \mathbf{u}) \simeq \bar{\mathbf{T}}_1 \cup \mathbf{K}_2$, where $\bar{\mathbf{T}}_1$ is a self-inverse tree on $n - 2$ vertices. Let $\mathbf{e} = (\mathbf{v}_1, \mathbf{v}_2)$ be any edge in the star underlying $\bar{\mathbf{S}}_n$. Then $\bar{\mathbf{S}}_n \setminus \mathbf{e} \simeq \bar{\mathbf{S}}_{n-2} \cup \mathbf{K}_2$. By induction $\bar{\mathbf{T}}_1 < \bar{\mathbf{S}}_{n-2}$, and hence $f_{\bar{\mathbf{T}}_1}(\lambda) \geq f_{\bar{\mathbf{S}}_{n-2}}(\lambda)$ holds for every $\lambda \geq \lambda(\bar{\mathbf{S}}_{n-2})$. The characteristic polynomial of the graph $\bar{\mathbf{T}}_1 \cup \mathbf{K}_2$ equals $(\lambda^2 - 1) \cdot f_{\bar{\mathbf{T}}_1}(\lambda)$ and that of $\bar{\mathbf{S}}_{n-2} \cup \mathbf{K}_2$ equals $(\lambda^2 - 1) \cdot f_{\bar{\mathbf{S}}_{n-2}}(\lambda)$. As $\lambda(\mathbf{G}) \geq 1$ for any graph with at least one edge, $f_{\bar{\mathbf{T}}_1}(\lambda) \geq f_{\bar{\mathbf{S}}_{n-2}}(\lambda)$ for every $\lambda \geq \lambda(\bar{\mathbf{S}}_{n-2})$ implies

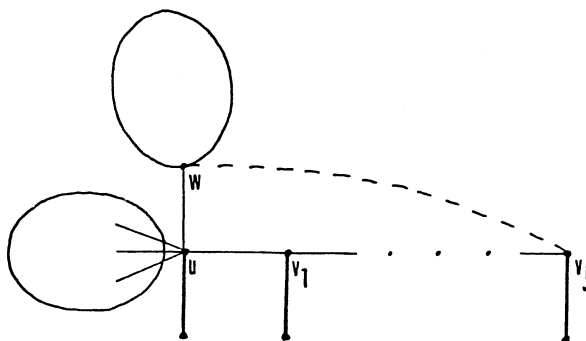


FIGURE 13.

$(\lambda^2 - 1) \cdot f_{\bar{T}}(\lambda) \geq (\lambda^2 - 1) \cdot f_{\bar{S}_{n-2}}(\lambda)$ for every $\lambda \geq \lambda(\bar{S}_{n-2})$, and hence $\bar{T} \setminus \{u, v\} \simeq \bar{T}_1 \cup K_2 < \bar{S}_{n-2} \cup K_2 \simeq \bar{S}_n \setminus e$.

On the other hand, $\bar{S}_n \setminus \{v_1, v_2\} \subset \subset \bar{T} \setminus \{w, u\}$ yields $(\bar{S}_n \setminus \{v_1, v_2\}) < (\bar{T} \setminus \{w, u\})$ by (ii). Hence $\bar{T} < \bar{S}_n$ by proposition (iii).

We have proved that $\bar{P}_n < \bar{T} < \bar{S}_n$. By (i) this implies $\lambda(\bar{P}_n) \leq \lambda(\bar{T}) \leq \lambda(\bar{S}_n)$. ■

In this way, we have proved the following theorem:

THEOREM 7 *Let T be a tree on n vertices. Then*

$$\lambda^+(\mathbf{T}) \leq \lambda^+(\bar{\mathbf{P}}_n).$$

Theorem 7 solves the problem of determining a graph on n vertices with the greatest λ^+ —it is \bar{P}_n . As noted above, the problem of determining a graph with the smallest λ^+ has been already solved by Godsil—the smallest λ^+ is obtained on the P_n . A direct corollary of Theorem 5 is that a graph with the second smallest λ^+ is Z_n :

THEOREM 8 *Let T be a tree on n vertices with a perfect matching, T nonisomorphic to P_n. Then*

$$\lambda^+(\mathbf{Z}_n) \leq \lambda^+(\mathbf{T}).$$

Summarizing, let T be a tree from Theorem 8. Then

$$\lambda^+(\mathbf{P}_n) < \lambda^+(\mathbf{Z}_n) \leq \lambda^+(\mathbf{T}) \leq \lambda^+(\bar{\mathbf{P}}_n).$$

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