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Note

On acyclic systems with minimal Hosoya index ☆

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Abstract

The Hosoya index of a graph is defined as the total number of independent edge subsets of the graph. In this note, we characterize the trees with a given size of matching and having minimal and second minimal Hosoya index. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

The *Hosoya index* of a graph originated from the work of Hosoya [5] in 1971 as a topological parameter to study the relation between molecular structure and physical and chemical properties of certain hydrocarbon compounds. Since then, much progress has been made in understanding the properties of Hosoya index and its applications by numerous investigators. A good survey may be found in [1,3,4].

Two edges of a graph G are said to be *independent* if they possess no vertex in common. Let $E(G)$ be the edge set of graph G. Any subset of $E(G)$ containing no two mutually incident edges is called an independent edge set. *Hosoya index* of a graph G is defined as the total number of independent edge sets of G, and denoted by $Z(G)$, that is,

$$Z(G)=\sum_{k=0} m(G,k), \tag{1}$$

where $m(G,k)$ denotes the number of ways in which k pairwise independent edges are selected in G, $k \geqslant 2$, in addition $m(G,0)=1$ and $m(G,1)=$ number of edges of

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the graph G. Recall that $m(G,k)$ is just the number of *k-matchings* of G and note that if $m(G,k)=0$, then necessarily $m(G,k+1)=0$. Besides, $m(G,k)=0$ whenever $k>n/2$. Therefore, the summations on the right-hand side of Eq. (1) go over a finite number of terms.

Among all n-vertex trees, the path P_n has the greatest Hosoya index and the star S_n has the smallest Hosoya index. This fact was established long time ago [2,4], that is, for any tree T with n vertices,

$$n=Z(S_n)\leqslant Z(T)\leqslant Z(P_n)=F_{n+1}, \tag{2}$$

where F_{n+1} is the $(n+1)$th Fibonacci number. Star with n vertices can be characterized within the set of all trees with n vertices by property: each matching contains only one edge ($n\geqslant 2$). Hence, in an improved inequality (2) for trees, it is natural to impose some lower bound on the size of a matching tree. In this note, we generalize the above lower bound for the trees with at least m-matchings.

Let k and r be non-negative integers, and let $n=2k+r+1$. We define a tree $S(n,k,r)$ with n vertices as follows: $S(n,k,r)$ is obtained from a star S with $k+r+1$ vertices by attaching a pendant edge to k non-central vertices. We call $S(n,k,r)$ a spur and note that it has a matching of $m=k+r'$ edges, where $r'=0$, if $r=0$ and $r'=1$, if $r>0$. Then the center of $S(n,k,r)$ is the center of the star S. For $m\geqslant 3$, let $R(n,k,r)$ be the graph obtained from the spur $S(n-2,k-1,r)$ by attaching a path of length 2 to one vertex of degree 2. Then $R(n,k,r)$ also has an m-matching, where $m=k+r'$ and $r'=0$ if $r=0$ and $r'=1$ if $r>0$. The center of $R(n,k,r)$ is the center of the spur $S(n-2,k-1,r)$. In Fig. 1, we have drawn $S(14,5,3)$ and $R(14,5,3)$.

We note that a spur $S(n,k,r)$ with $k>0$ has at least two m-matchings unless $r=1$. In the case $r=1$, $m=k+1=\frac{1}{2}n$, and m-matching is a perfect matching in the sense that each vertex is incident to an edge of the matching. It is easy to prove by induction that a perfect matching of a tree is unique when it exists.

Our main result is

Theorem 1. *Let T be an n-vertex tree with an m-matching, where $m\geqslant 1$. Then*

$$Z(T)\geqslant 2^{m-2}(2n-3m+3)$$

with equality if and only if T is the spur $S(n,m-1,n-2m+1)$ (see Fig 1).

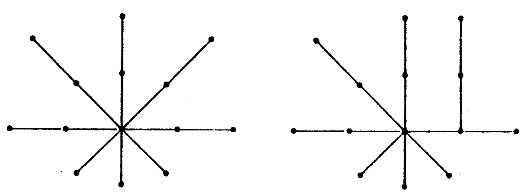

Fig. 1. The graphs of $S(14,5,3)$ and $R(14,5,3)$.

2. Proofs

Let T be an n-vertex tree and A be its *adjacency matrix*. We call the matrix $I+A$ the *neighbor matrix* of T and write $B(T)=I+A$, where I is the unit matrix of order n. Recall the definition of *permanent* [7] of a matrix $B=(b_{ij})$,

$$per(B)=\sum_{\sigma}\prod_{i=1}^{n} b_{i\sigma(i)}, \tag{3}$$

where the summation is taken over the symmetric group of order n. Since the tree T has no cycles, $\prod_{i=1}^{n} b_{i\sigma(i)}=0$ if σ has a cycle of length 3 or more. For permutations σ containing cycles of length at the most 2, $\prod_{i=1}^{n} b_{i\sigma(i)}=0$ if for some $i\neq\sigma(i)$, $v_i v_{\sigma(i)}\notin E(T)$. This gives the following:

Lemma 1. *Let T be a tree. Then*

$$Z(T)=per(I+A).$$

In order to obtain the proof of Theorem 1 we need the following structure properties of trees. In what follows, we use the notation $v\in M$ to mean that the vertex v is incident with some edge in M, and $v\notin M$ means that the vertex v is not incident with any edge in M.

Lemma 2. *Let T be an n-vertex tree with a perfect matching. Then T has a pendant edge which is incident to a vertex of degree* 2.

Proof. We need only root T at a vertex r and choose a pendant vertex v farthest from r. Let $e=vw$ be the unique pendant edge incidenting the vertex v. If the degree of the vertex w is not 2, then there would be a pendant vertex $u\neq v$ joined to w. This contradicts with T having a perfect matching. □

Lemma 3. *Let T be an n-vertex tree with an m-matching where $n>2m$. Then there is an m-matching M and a pendant vertex v such that $v\notin M$.*

Proof. For $n\leqslant 3$ the result clearly holds. We assume that $n>3$ and proceed by induction. Let $\bar{M}$ be an m-matching of an n-vertex tree T. Root T is at a vertex r and let v be a pendant vertex farthest from r. Let vw be the unique pendant edge incidenting the vertex v. If vw does not belong to $\bar{M}$, then the conclusion follows. So we may assume that vw belongs to $\bar{M}$. If the degree of w is not 2, then there is a pendant vertex $\bar{v}\neq v$ joined to w and $\bar{v}\notin\bar{M}$. Thus, we may assume that w has degree 2. Let ww' be an edge with $w'\neq v$, and let T' be the tree obtained from T by removing vertices v, w and edges vw and ww'. Then T' has $n-2=n'$ vertices and an m'-matching, where $m'=m-1$. Since $n'>2m'$, it follows by induction that T' has an m'-matching M' and a pendant vertex v' such that $v'\notin M'$. If $v'\neq w'$, then $M''=M'\cup\{vw\}$ is an m-matching of T such that the pendant vertex $v'\notin M'$. If

$v' = w'$, then $M'' = M' \cup \{v'w\}$ is an m-matching such that the pendant vertex $v \notin M''$. Hence, the lemma holds by induction. □

We now compute the Hosoya index of the spur $S(n,k,r)$ in the following lemma:
Lemma 4.

$$Z(S(n,k,r)) = 2^{k-1}(2r + k + 1). \tag{4}$$

Proof. We can order the vertices of $S(n,k,r)$ such that its neighboring matrix is

$$\begin{array}{c} \qquad \overbrace{\hphantom{1\ \ 0\ \ \cdots\ \ 1\ \ 0}}^{2k}\ \ \overbrace{\hphantom{1\ \ \cdots\ \ 1}}^{r} \\ \begin{bmatrix} 1 & 1 & 0 & \cdots & 1 & 0 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 1 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ \vdots & & & \ddots & & & & & \\ 1 & & & & 1 & 1 & & & \\ 0 & & & & 1 & 1 & & & \\ 1 & & & & & & 1 & & \\ \vdots & & & & & & & \ddots & \\ 1 & & & & & & & & 1 \end{bmatrix} \end{array},$$

where the unwritten entries are all zeros. Calculating the permanent by an expansion along the first row, we then obtain

$$Z(S(n,k,r)) = per\, B(S(n,k,r)) = 2^k + k2^{k-1} + r2^k = 2^{k-1}(2r + k + 2). \qquad \square$$

Proof of Theorem 1. Since T has an m-matching, $n \geqslant 2m$. First we suppose that $n = 2m$, that is, T has a perfect matching. We prove that $Z(T) \geqslant 2^{m-2}(m+3)$ and with equality if and only if T is the spur $S(2m, m-1, 1)$ by induction on m. If $m = 1$ or 2, then T must be the spur $S(2m, m-1, 1)$, since T has a perfect matching. We now suppose that $m \geqslant 3$ and proceed by induction. By Lemma 2, T has a pendant edge vw which is incident on a vertex w of degree 2. Thus, there exists a unique vertex $u \neq v$ such that we is an edge. Let T' be the tree with $2(m-1)$ vertices and with an $(m-1)$-matching obtained from T by deleting vertices v and w and edges vw and we. By the inductive assumption

$$Z(T') \geqslant 2^{m-3}(m - 1 + 3) \tag{5}$$

with equality if and only if T' is the spur $S(2m-2, m-2, 1)$. Ordering the vertices of T as $v, w, u, \ldots$, then

$$B(T) = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & x \\ 0 & 0 & x^T & C \end{bmatrix}, \quad B(T') = \begin{bmatrix} 1 & x \\ x^T & C \end{bmatrix}.$$

So a simple calculation gives

$$Z(G) = per\,B(T) = per\,C + 2\ per\,B(T') = per\,C + 2Z(T'). \tag{6}$$

Since T' has a perfect matching of $m-1$ edges, then with a suitable ordering of its vertices, C has the form

$$\begin{bmatrix} 1 & 1 & & & * & \\ 1 & 1 & & & & \\ & & \ddots & & & \\ * & & & 1 & 1 & \\ & & & 1 & 1 & \\ & & & & & 1 \end{bmatrix},$$

where there are $(m-2)$ blocks

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

in C. Thus,

$$per\,C \geqslant 2^{m-2}. \tag{7}$$

Combining (5)–(7), and Lemma 1, we have

$$\begin{aligned} Z(T) = per\,B(T) &\geqslant 2^{m-2} + 2 \times 2^{m-3}(m-1+3) \\ &= 2^{m-2}(m+3) = Z(S(2m, m-1, 1)). \end{aligned} \tag{8}$$

Suppose that equality holds in (8). Then equality holds in (5) and it follows by the inductive assumption that T' is the spur $S(2m-2, m-2, 1)$. Moreover, if equality holds in (7), then we conclude that the entries in $(*)$ of C are zero. From this it follows that the vertex u is the center of spur $S(2m-2, m-2, 1)$, and hence that T is the spur $S(2m, m-1, 1)$. This completes the induction on m and completes the proof of theorem when $n = 2m$.

We now suppose that $n > 2m$ and proceed by induction on n. By Lemma 3, T has an m-matching M and a pendant vertex v such that $v \notin M$. Let w be the unique vertex such that vw is an edge and T' be the tree obtained from T by removing the vertex v and the edge vw. Then T' has $n-1$ vertices and has an m-matching. By the induction assumption

$$Z(T') \geqslant 2^{m-2}[2(n-1) - 3m + 3] = 2^{m-2}(2n - 3m + 1) \tag{9}$$

with equality if and only if T' is the spur $S(n-1, m-1, n-2m)$. Ordering the vertices of T as $v, w, \ldots$, we obtain

$$B(T) = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & x \\ 0 & x^{\mathrm{T}} & C \end{bmatrix}, \quad B(T') = \begin{bmatrix} 1 & x \\ x^{\mathrm{T}} & C \end{bmatrix}.$$

By expanding the permanent along the first row, we have

$$per\,B(T) = per\,B(T') + per\,C,$$

that is,

$$Z(T) = Z(T') + per\, C. \tag{10}$$

Since T' has an m-matching, it follows as in the previous induction that

$$per\, C \geqslant 2^{m-1}. \tag{11}$$

Combining (9), (10), (11), and Lemma 1, we obtain

$$\begin{aligned} Z(T) &\geqslant 2^{m-1} + 2^{m-2}(2n - 3m + 1) \\ &= 2^{m-2}(2n - 3m + 2) = Z(S(n, m-1, n-2m+1)). \end{aligned} \tag{12}$$

If the equality in (12) holds, then inequalities (9) and (11) become equalities. By the inductive assumption T' is the spur $S(n-1, m-1, n-2m)$. It again follows as in the previous induction that vertex w is the center of $S(n-1, m-1, n-2m)$, and hence T is the spur $S(n, m-1, n-2m+1)$. Thus, the theorem is proved by induction. □

As an analogue to $S(n, m-1, n-2m+1)$, we can obtain

$$Z(R(n, m-1, n-2m+1)) = 5(2n - 3m)2^{m-4},$$

and similar to the above proof of Theorem 1, we can prove the following:

Theorem 2. *Let T be an n-vertex tree with an m- matching where $m \geqslant 1$, and $T \neq S(n, m-1, n-2m+1)$. Then*

$$Z(T) \geqslant 5(2n - 3m)2^{m-4}$$

with equality if and only if T is $R(n, m-1, n-2m+1)$ (see Fig. 1).

While we have determined the minimum value of the Hosoya indices of n-vertex trees with an m-matching, the maximum Hosoya indices with constraints corresponding to those imposed for the minimum value seems more difficult, although the path P_n has a maximum Hosoya index when $n = 2m$. Another interesting problem is to determine the minimum (maximum) value of the Hosoya indices of n-vertex chemical trees (trees which have no vertices with degrees > 3) with an m-matching, although the comb graph C_n has a minimum Hosoya index when $n = 2m$ [6,8].

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