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On the Hosoya index of trees

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It is well known that the Hosoya index is important in structural chemistry. In [4], authors found a relation between Hosoya index of a tree and eigenvalues of its adjacency matrix. In this paper we give a relation between Hosoya index of a tree and the coefficients of characteristic polynomial of its adjacency matrix.

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1. Introduction

Let G be a connected simple graph with *m* edges and *n* vertices. The adjacency matrix of G is an $n \times n$ matrix $A = (a_{i,j})$ in which the entry $a_{i,j} = 1$ if there is an edge from vertex *i* to vertex *j* and is *0* if there is no edge from vertex *i* to vertex *j*.

If A is an $n \times n$ matrix, then a nonzero vector x is called an eigenvector of *A* if Ax is a scalar multiple of n; that is, $Ax = \lambda x$ for some scalar λ. The scalar λ is called an eigenvalue of A and x is said to be an eigenvector corresponding to λ. [8]

To find the eigenvalues of an $n \times n$ matrix A we rewrite $Ax - \lambda x$ as $(\lambda I - A)x - 0$. Scalar λ is an eigenvalue of A if and only if $\det(\lambda I - A) = 0$.

It can be shown that the determinant $\det(\lambda I - A)$ is a polynomial in λ that called the characteristic polynomial of A, i.e. $\det(\lambda I - A) = \lambda^n + a_{n-1}\lambda^{n-1} + \cdots + a_0$.

We represent the characteristic polynomial of A by $P_n(\lambda)$. The eigenvalues of A are the roots of $P_n(\lambda)=0$.

The Hosoya index, also known as the Z index, of a graph is the total number of matchings in it. A k-matching of the graph G is the set of k edges of that graph which are independent; that is, none of these k edges are adjacent to each other. The Hosoya index is always at least one, because the empty set of edges is counted as a matching for this purpose. Equivalently, the Hosoya index is the number of non-empty matchings plus one. This graph invariant was introduced by Haruo Hosoya in 1971. It is often used in chemoinformatics for investigations of organic compounds.

The Hosoya index of trees is directly related to the graph eigenvalues by $Z = \prod_{j=1}^{n}\sqrt{1+\lambda_j^2}$ [4]. The present paper aims to prove, by the use of the above relation and Vieta's formula, that for trees, Z index is equal to the sum of absolute value of the coefficients of characteristic polynomial of the adjacency matrix.

Vieta's formula [6]

Let s_i be the sum of the products of distinct polynomial roots λ_j of the polynomial equation of degree n

$$p_n(\lambda) = \lambda^n + a_{n-1}\lambda^{n-1} + \cdots + a_0 \tag{1}$$

where the roots are taken i at a time. The first few values of s_i are

$$s_1 = \sum_{i=1}^{n}\lambda_i = \lambda_1 + \cdots + \lambda_n$$

$$s_2 = \sum_{1\le i<j\le n}\lambda_i\lambda_j = \lambda_1\lambda_2 + \lambda_1\lambda_3 + \cdots + \lambda_1\lambda_n + \lambda_2\lambda_3 + \cdots + \lambda_{n-1}\lambda_n$$

$$s_3 = \sum_{1\le i<j<k\le n}\lambda_i\lambda_j\lambda_k = \lambda_1\lambda_2\lambda_3 + \lambda_1\lambda_2\lambda_4 + \cdots + \lambda_1\lambda_2\lambda_n + \lambda_2\lambda_3\lambda_4 + \cdots + \lambda_{n-2}\lambda_{n-1}\lambda_n$$

and so on. Then Vieta's formulas states that $s_i = (-1)^i a_{n-i}$.

2. Main results and discussion

In this paper we prove that sum of absolute value of the coefficient of characteristic polynomial of the adjacency matrix of a tree is equals to Z index. In order to prove this, we need the following lemmas.

Lemma1: Let $\lambda_1, \ldots, \lambda_n$ be the roots of characteristic polynomial of a tree, then

$$\lambda_1 = -\lambda_n, \lambda_2 = -\lambda_{n-1}, \cdots, \lambda_{\left[\frac{n+1}{2}\right]} = -\lambda_{\left[\frac{n}{2}\right]+1}$$

Proof: [4], [5].

Lemma 2: Let $p_n(\lambda) = \lambda^n + a_{n-1}\lambda^{n-1} + \cdots + a_0$ be the characteristic polynomial of a tree, then the coefficients of $p_n(\lambda)$ are zero alternately. i.e.

$$P_n(\lambda) = \begin{cases} \lambda^n + a_{n-2}\lambda^{n-2} + \cdots + a_0 & n \text{ is even} \\ \lambda^n + a_{n-2}\lambda^{n-2} + \cdots + a_1\lambda & n \text{ is odd} \end{cases}$$

Proof: There are two cases:

Case 1: The number of the vertices of the tree is even.

Let $\lambda_1, \dots, \lambda_n$ be the eigenvalues of the tree. In this case by lemma 1, we have

$P_n(\lambda) = \prod_{i=1}^{n}(\lambda - \lambda_i)$

$=(\lambda - \lambda_1)(\lambda + \lambda_1)(\lambda - \lambda_2)(\lambda + \lambda_2)\dots\left(\lambda - \lambda_{\frac{n}{2}}\right)(\lambda + \lambda_{\frac{n}{2}})$

$=\prod_{i=1}^{\frac{n}{2}}(\lambda^2 - \lambda_i^2)$

Therefore, the coefficients of λ with odd powers are zero.

Case 2: The number of the vertices of the tree is odd.

Suppose that $n = 2k + 1$. In this case by lemma 1, $\lambda_{k+1} = 0$ and we have

$$P_n(\lambda) = \prod_{j=1}^{2k}(\lambda - \lambda_j)\lambda = \prod_{j=1}^{k}(\lambda^2 - \lambda_j^2)\lambda$$

So the power of λ in all term of P_n (λ) is odd, i.e., the coefficient of λ with even power equals zero. In this case, the constant coefficient will be zero, too.

Lemma 3: Non-zero coefficients of characteristic polynomial of a tree are positive and negative alternately.

Proof: Suppose that $\lambda_1, \dots, \lambda_n$ are the roots of characteristic polynomial $P_n(\lambda) = 0$.

There are two cases:

Case 1: $n = 2k$ (n is even).

In this case by lemma 1 and lemma 2, we have

$$P_n(\lambda) = \lambda^n + a_{n-2}\lambda^{n-2} + \cdots + a_0 = (\lambda - \lambda_1)(\lambda - \lambda_2)\dots(\lambda - \lambda_n) = \prod_{i=1}^{k}(\lambda^2 - \lambda_i^2) \qquad (2)$$

The coefficient of λ^n is 1 and the coefficient of λ^{n-2} is $-\sum_{i=1}^{k}\lambda_i^2$, thus $a_{n-2} = -\sum_{i=1}^{k}\lambda_i^2 < 0$. According to (2), it is not difficult to see that a_{n-2l} is negative if l is odd and is positive if l is even.

Case 2: $n = 2k + 1$ (n is odd).

In this case, we have

$P_n(\lambda) = \lambda^n + a_{n-2}\lambda^{n-2} + \cdots + a_1\lambda = \prod_{j=1}^{k}(\lambda^2 - \lambda_j^2)\lambda$

and similar to case 1, we obtain the same result.

Theorem: Let $p_n(\lambda) = \lambda^n + a_{n-1}\lambda^{n-1} + \cdots + a_0$ be the characteristic polynomial of a tree, then

$$Z = 1 + \sum_{i=0}^{n-1}|a_i|.$$

Proof: In [4], authors proved that the value of Z index for a tree is equal to $\prod_{j=1}^{n}\sqrt{1 + \lambda_j^2}$. Hence we show that

$\sum_{i=0}^{n}|a_i| = \prod_{j=1}^{n}\sqrt{1 + \lambda_j^2}$.

There are two cases:

Case 1: $n = 2m$, i.e., n is even.

According to lemma 1, we have

$\prod_{j=1}^{n}\sqrt{1 + \lambda_j^2} = \prod_{j=1}^{m}(1 + \lambda_j^2)$.

First, we prove

$$\prod_{j=1}^{m}(1 + \lambda_j^2) = 1 + \sum_{i=1}^{m}\lambda_i^2 + \sum_{1\le i<j\le m}\lambda_i^2\lambda_j^2 + \cdots + \prod_{i=1}^{m}\lambda_i^2 \qquad (3)$$

by induction on the m.

For $m = 2$ and $m = 3$, we have

$(1 + \lambda_1^2)(1 + \lambda_2^2) = 1 + \lambda_1^2 + \lambda_2^2 + \lambda_1^2\lambda_2^2$

$(1 + \lambda_1^2)(1 + \lambda_2^2)(1 + \lambda_3^2) = (1 + \lambda_1^2 + \lambda_2^2 + \lambda_1^2\lambda_2^2)(1 + \lambda_3^2) =$

$1 + \lambda_1^2 + \lambda_2^2 + \lambda_3^2 + \lambda_1^2\lambda_2^2 + \lambda_1^2\lambda_3^2 + \lambda_2^2\lambda_3^2 + \lambda_1^2\lambda_2^2\lambda_3^2$

Suppose that (3) is true for $m = k - 1$, i.e.,

$\prod_{j=1}^{k-1}(1 + \lambda_j^2) = 1 + \sum_{i=1}^{k-1}\lambda_i^2 + \sum_{1\le i<j\le k-1}\lambda_i^2\lambda_j^2 + \cdots + \prod_{i=1}^{k-1}\lambda_i^2$.

For $m = k$, we have

$$\prod_{j=1}^{k}(1 + \lambda_j^2) = \prod_{j=1}^{k-1}(1 + \lambda_j^2)(1 + \lambda_k^2) = (1 + \sum_{i=1}^{k-1}\lambda_i^2 + \sum_{1\le i<j\le k-1}\lambda_i^2\lambda_j^2 + \cdots\prod_{i=1}^{k-1}\lambda_i^2)(1 + \lambda_k^2) =$$
$$1 + \sum_{i=1}^{k-1}\lambda_i^2 + \sum_{1\le i<j\le k-1}\lambda_i^2\lambda_j^2 + \cdots + \prod_{i=1}^{k-1}\lambda_i^2 + \lambda_k^2 + \sum_{i=1}^{k-1}\lambda_i^2\lambda_k^2 + \sum_{1\le i<j\le k-1}\lambda_i^2\lambda_j^2\lambda_k^2 + \cdots + \prod_{i=1}^{k}\lambda_i^2. \qquad (4)$$

By rearranging (4), we have

$$\prod_{j=1}^{k}(1 + \lambda_j^2) = 1 + \sum_{i=1}^{k}\lambda_i^2 + \sum_{1\le i<j\le k}\lambda_i^2\lambda_j^2 + \cdots + \prod_{i=1}^{k}\lambda_i^2 \qquad (5)$$

Now we intend to show that the relation (5) is equal to the sum of absolute value of the coefficients of characteristic polynomial having roots $\lambda_1, \lambda_2, \dots, \lambda_n$.

Case 1: $n = 2k$

By lemma 1 and lemma 2, we have

$p_n(\lambda) = \lambda^n + a_{n-1}\lambda^{n-1} + \cdots + a_0 = \prod_{i=1}^{k}(\lambda^2 - \lambda_i^2)$.

By replacing $\lambda^2 = t$, we have

$P_k(t) = t^k + a_{n-2}t^{k-1} + a_{n-4}t^{k-2} + \cdots + a_0$

whose roots are equal to $\lambda_1^2, \lambda_2^2, \dots, \lambda_k^2$ and whose coefficients are $1, a_{n-2}, a_{n-4}, \dots, a_0$ respectively.

Using Vieta's formula for $P_k(t)$, we have

$$\sum_{i=1}^{k} \lambda^2{}_i = -a_{n-2}$$
$$\sum_{1 \le i < j \le k} \lambda_i^2 \lambda_j^2 = a_{n-4}$$
$$\vdots$$
$$\prod_{i=1}^{k} \lambda_i^2 = (-1)^k a_0$$

and since the coefficients of characteristic polynomial of the tree are zero alternately, therefore,

$$1 + |a_{n-1}| + |a_{n-2}| + \cdots + |a_0| = 1 + |a_{n-2}| + |a_{n-4}| + \cdots + |a_0| \quad (6)$$

Also by lemma 3, $a_{n-2}, a_{n-6}, a_{n-10}, \ldots$ are negative, so,

$$1 + |a_{n-1}| + |a_{n-2}| + \cdots + |a_0| = 1 - a_{n-2} + a_{n-4} - a_{n-6} + \cdots \pm a_0$$

Using Vieta's formula and (6), we obtain

$$1 + \sum_{i=0}^{n-1} |a_i| = 1 + \sum_{i=1}^{k} \lambda_i^2 + \sum_{1 \le i < j \le k} \lambda_i^2 \lambda_j^2 + \cdots + \prod_{i=1}^{k} \lambda_i^2 \quad (7)$$

By (5) and (7)

$$Z = 1 + \sum_{i=0}^{n-1} |a_i| .$$

Case 2: $n = 2k+1$, i.e., n is odd.

In this case, by lemma 1, $\lambda_{k+1} = 0$, and so

$$\prod_{j=1}^{n} \sqrt{1 + \lambda_j^2} = \prod_{j=1}^{k} (1 + \lambda_j^2) ,$$

$$P_n(\lambda) = (\lambda - \lambda_1)(\lambda - \lambda_2) \ldots (\lambda - \lambda_k)\lambda(\lambda - \lambda_{k+2}) \ldots (\lambda - \lambda_n) = \lambda(\lambda^2 - \lambda_1^2)(\lambda^2 - \lambda_2^2) \ldots (\lambda^2 - \lambda_k^2)$$

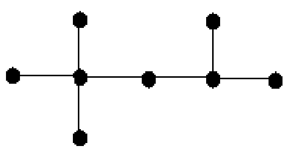
whose roots will be equal to $\lambda_1^2, \lambda_2^2 \ldots, \lambda_k^2$. By changing the variable $\lambda^2 = t$ and replacing $x^i = t^i \lambda$, we have

$$P_n(\lambda) = \lambda(\lambda^{2k} + a_{n-2}\lambda^{2k-2} + \cdots + a_1)$$
$$P_k(x) = x^k + a_{n-2}x^{k-1} + a_{n-4}x^{k-2} + \cdots + a_1$$

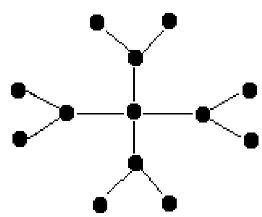
whose roots are $\lambda_1^2, \lambda_2^2, \ldots, \lambda_k^2$. In this case, similar to case 1, we obtain the same result.

3. Numerical example

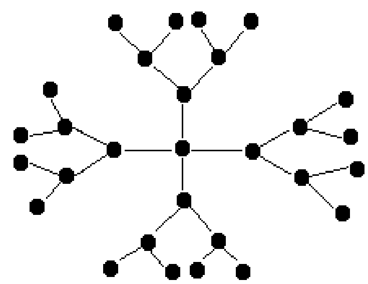
Consider the following trees. The Hosoya index for them is available in table 1.



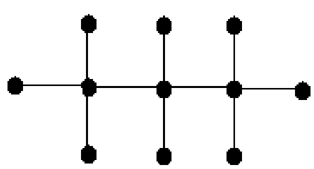
T1



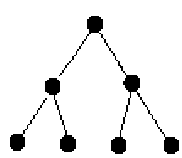
T2



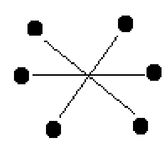
T3



T4



T5



T6

Table 1

Trees	The non-zero coefficients of characteristic polynomial										$Z = \sum_{i=0}^{n} \lvert a_i \rvert$
T1	1	-7	11								19
T2	1	-12	48	-80	48						189
T3	1	-28	336	-2272	9552	-25920	45440	-49664	30720	-8192	172125
T4	1	-10	27	-18							56
T5	1	-6	8								15
T6	1	-6									7

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