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An Upper Bound for the Hosoya Index of Trees

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Abstract

The Hosoya index of a graph G is defined as the sum of all the numbers of k - matchings ($k \geq 0$) in G. An upper bound for the Hosoya index of trees is presented in this note.

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We consider only finite undirected graphs without loops or multiple edges. Notation and terminology not defined here follow that in [1]. Let G be a graph of order n. We assume that d_1, d_2, ..., d_n, where d_i, $1 \leq i \leq n$, is the degree of vertex v_i in G, is the degree sequence of G. For each vertex v_i, $1 \leq i \leq n$, we use t_i to denote the 2 - degree of vertex v_i, which is the sum of degrees of the vertices adjacent to vertex v_i. Moreover, we use N_i to denote the sum of 2 - degrees of vertices adjacent to v_i. We define $\Sigma_k(G)$ as $\sum_{i=1}^{n} d_i^k$. Obviously, $\Sigma_{i=1}^{n} t_i = \Sigma_{i=1}^{n} d_i^2 = \Sigma_2(G)$. A bipartite graph is called *semiregular* if all the vertices in the same part of a bipartition have the same degree. The Hosoya index of a graph G was introduced by Hosoya in [4] and it is defined as $Z(G) = \sum_{k \geq 0} m(G, k)$, where $m(G, k)$ is the number of k - matchings in G. Notice that $m(G, 0) = 1$. The eigenvalues $\mu_1(G) \geq \mu_2(G), ..., \geq \mu_n(G)$ of a graph G are defined as the eigenvalues of $A(G)$, the adjacency matrix of G.

The objective of this note is to prove the following theorem in which we provide an upper bound for the Hosoya index of trees.

Theorem 1. Let T be a tree of $n \geq 3$ vertices and let $f(x)$ be $(1 + x^2)^2(3n -$

$4-2x^2)^{n-2}$. Then

$$Z(T) \leq \sqrt{\frac{f(\sqrt{\frac{\sum_{i=1}^{n} N_i^2}{\sum_{i=1}^{n} t_i^2}})}{(n-2)^{(n-2)}}}$$

with equality if and only if at least one of the following statements is true:

(1) T is $K_{1,n-1}$.

(2) $\frac{N_1}{t_1} = \frac{N_2}{t_2} = ... = \frac{N_n}{t_n}$ and T has eigenvalues $\mu_1 = \frac{N_1}{t_1}$, $\mu_n = -\mu_1$, $\mu_i = \sqrt{\frac{2(n-1-\mu_1^2)}{n-2}}$ for each i with $2 \leq i \leq r$, and $\mu_j = -\sqrt{\frac{2(n-1-\mu_1^2)}{n-2}}$ for each j with $r+1 \leq j \leq n-1$, where r is some integer such that $2 \leq r \leq n-2$.

(3) T is a bipartite graph with $V(T) = V_1 \cup V_2$, where $V_1 = \{ v_1, v_2, ..., v_s \}$ and $V_2 = \{ v_{s+1}, v_{s+2}, ..., v_n \}$ such that $\frac{N_1}{t_1} = \frac{N_2}{t_2} = ... = \frac{N_s}{t_s}$ and $\frac{N_{s+1}}{t_{s+1}} = \frac{N_{s+2}}{t_{s+2}} = ... = \frac{N_n}{t_n}$, and T has eigenvalues $\mu_1 = \sqrt{\frac{\sum_{i=1}^{n} N_i^2}{\sum_{i=1}^{n} t_i^2}}$, $\mu_n = -\mu_1$, $\mu_i = \sqrt{\frac{2(n-1-\mu_1^2)}{n-2}}$ for each i with $2 \leq i \leq r$, and $\mu_j = -\sqrt{\frac{2(n-1-\mu_1^2)}{n-1}}$ for each j with $r+1 \leq j \leq n-1$, where r is some integer such that $2 \leq r \leq n-2$.

In order to prove Theorem 1, We need the following theorems.

Theorem 2. [2] Let T be a tree of n vertices and $\mu_1(T) \geq \mu_2(T), ..., \geq \mu_n(T)$ are eigenvalues of T. Then

$$Z(T) = \prod_{i=1}^{n} \sqrt{1+\mu_i^2}.$$

Theorem 3. [3] Let G be a simple connected graph of order n. Then

$$\mu_1 \geq \sqrt{\frac{\sum_{i=1}^{n} N_i^2}{\sum_{i=1}^{n} t_i^2}}$$

with equality if and only if $\frac{N_1}{t_1} = \frac{N_2}{t_2} = ... = \frac{N_n}{t_n}$ or G is a bipartite graph with $V(G) = V_1 \cup V_2$, $V_1 = \{ v_1, v_2, ..., v_s \}$, and $V_2 = \{ v_{s+1}, v_{s+2}, ..., v_n \}$ such that $\frac{N_1}{t_1} = \frac{N_2}{t_2} = ... = \frac{N_s}{t_s}$ and $\frac{N_{s+1}}{t_{s+1}} = \frac{N_{s+2}}{t_{s+2}} = ... = \frac{N_n}{t_n}$.

Theorem 4. [5] Let T be a tree of n vertices. Then $\mu_1(G) \leq \sqrt{n-1}$, and equality holds if and only if T is $K_{1,n-1}$.

Proof of Theorem 1. Since T is a tree, T is a bipartite graph and therefore $\mu_1 = -\mu_n$. Thus by Theorem 2 and the inequality for arithmetic and geometric means we have that

$$(Z(T))^2 = (1+\mu_1^2)^2 \prod_2^{n-1}(1+\mu_i^2) \le (1+\mu_1^2)^2 \frac{(\sum_2^{n-1}(1+\mu_i^2))^{n-2}}{(n-2)^{n-2}}$$
$$= \frac{(1+\mu_1^2)^2(n-2+\sum_1^n \mu_i^2 - 2\mu_1^2)^{n-2}}{(n-2)^{n-2}}$$
$$= \frac{(1+\mu_1^2)^2(n-2+2|E(H)|-2\mu_1^2)^{n-2}}{(n-2)^{n-2}}$$
$$= \frac{(1+\mu_1^2)^2(3n-4-2\mu_1^2)^{n-2}}{(n-2)^{n-2}}.$$

Now consider the function $f(x) = (1+x^2)^2(3n-4-2x^2)^{n-2}$. It can be easily checked that $f(x)$ is decreasing when $\sqrt{\frac{3n-4}{2}} \ge x \ge \sqrt{\frac{2(n-1)}{n}}$.

Recall that, for a connected graph G, Hong and Zhang proved the following inequality in [3]

$$\mu_1 \ge \sqrt{\frac{\sum_{i=1}^n N_i^2}{\sum_{i=1}^n t_i^2}} \ge \sqrt{\frac{\sum_{i=1}^n t_i^2}{\sum_{i=1}^n d_i^2}}.$$

Recall again that, for a connected graph G, Yu, Lu, and Tian proved the following inequalities in [6]

$$\sqrt{\frac{\sum_{i=1}^n t_i^2}{\sum_{i=1}^n d_i^2}} \ge \sqrt{\frac{\sum_{i=1}^n d_i^2}{n}} \ge \frac{2|E(G)|}{n}.$$

Therefore, for the tree T, we have the following inequalities

$$\mu_1 \ge \sqrt{\frac{\sum_{i=1}^n N_i^2}{\sum_{i=1}^n t_i^2}} \ge \sqrt{\frac{\sum_{i=1}^n t_i^2}{\sum_{i=1}^n d_i^2}} \ge \sqrt{\frac{\sum_{i=1}^n d_i^2}{n}}$$
$$\ge \frac{2|E(T)|}{n} = \frac{2(n-1)}{n} \ge \sqrt{\frac{2(n-1)}{n}}.$$

From Theorem 4, we have that $\mu_1 \le \sqrt{n-1} \le \sqrt{\frac{3n-4}{2}}$.

Hence

$$f(\mu_1) \le f(\sqrt{\frac{\sum_{i=1}^n N_i^2}{\sum_{i=1}^n t_i^2}}).$$

So

$$Z(T) \le \sqrt{\frac{f(\mu_1)}{(n-2)^{(n-2)}}} \le \sqrt{\frac{f(\sqrt{\frac{\sum_{i=1}^n N_i^2}{\sum_{i=1}^n t_i^2}})}{(n-2)^{(n-2)}}}.$$

If T is $K_{1,n-1}$, a simple calculation shows that both sides of the inequality in this theorem are equal to n. If T is a tree satisfying the conditions in (2) of this theorem, then by Theorem 3, we have that $\mu_1 = \sqrt{\frac{\sum_{i=1}^{n} N_i^2}{\sum_{i=1}^{n} t_i^2}}$. Since $\frac{N_1}{t_1} = \frac{N_2}{t_2} = ... = \frac{N_n}{t_n}$, $\mu_1 = \frac{N_1}{t_1}$. A simple calculation shows that both sides of the inequality in this theorem are the same. If T is a tree satisfying the conditions in (3) of this theorem, then again by Theorem 3, we have that $\mu_1 = \sqrt{\frac{\sum_{i=1}^{n} N_i^2}{\sum_{i=1}^{n} t_i^2}}$. A simple calculation shows that both sides of the inequality in this theorem are the same.

Now suppose that the inequality in this theorem becomes equality. Reviewing the above proof of the inequality in this theorem, we have that $|\mu_2| = |\mu_3| = ... = |\mu_{n-1}|$ and $\mu_1 = \sqrt{\frac{\sum_{i=1}^{n} N_i^2}{\sum_{i=1}^{n} t_i^2}}$. Then Theorem 3 implies that $\frac{N_1}{t_1} = \frac{N_2}{t_2} = ... = \frac{N_n}{t_n}$ or T is a bipartite graph with $V(T) = V_1 \cup V_2$, where $V_1 = \{ v_1, v_2, ..., v_s \}$ and $V_2 = \{ v_{s+1}, v_{s+2}, ..., v_n \}$ such that $\frac{N_1}{t_1} = \frac{N_2}{t_2} = ... = \frac{N_s}{t_s}$ and $\frac{N_{s+1}}{t_{s+1}} = \frac{N_{s+2}}{t_{s+2}} = ... = \frac{N_n}{t_n}$. Then we have the following cases.

Case 1. There exists an i, where $2 \leq i \leq (n-1)$, such that $|\mu_i| = 0$.

In this case, we have that $\mu_2 = \mu_3 = ... = \mu_{n-1} = 0$. Since $\sum_{i=1}^{n} \mu_i^2 = 2|E(T)|$ and $\mu_1 = -\mu_n$, $\mu_1 = \sqrt{|E(T)|} = \sqrt{n-1}$. By Theorem 4, we have that T is $K_{1,n-1}$.

Case 2. For any i, where $2 \leq i \leq (n-1)$, we have that $|\mu_i| \neq 0$.

If $\mu_2 \geq \mu_3 \geq ... \geq \mu_{n-1} \geq 0$ or $0 \geq \mu_2 \geq \mu_3 \geq ... \geq \mu_{n-1}$, then by $\sum_{i=1}^{n} \mu_i = 0$ we have that $\mu_2 = \mu_3 = ... = \mu_{n-1} = 0$, contradicting to the assumption of this case. Thus there exists an integer r such that $\mu_2 \geq \mu_3 \geq ... \geq \mu_r > 0 > \mu_{r+1} \geq \mu_{r+2} \geq ... \geq \mu_{n-1}$, where $2 \leq r \leq n-2$.

Now if $\frac{N_1}{t_1} = \frac{N_2}{t_2} = ... = \frac{N_n}{t_n}$, then $\mu_1 = \frac{N_1}{t_1}$ and $\mu_n = -\mu_1 = -\frac{N_1}{t_1}$. From $\sum_{i=1}^{n} \mu_i^2 = 2|E(T)| = 2(n-1)$, we have that $\mu_i = \sqrt{\frac{2(n-1-\mu_1^2)}{n-2}}$, where $2 \leq i \leq r$, and $\mu_j = -\sqrt{\frac{2(n-1-\mu_1^2)}{n-2}}$, where $r+1 \leq j \leq n-1$.

If T is a bipartite graph with $V(T) = V_1 \cup V_2$, where $V_1 = \{ v_1, v_2, ..., v_s \}$ and $V_2 = \{ v_{s+1}, v_{s+2}, ..., v_n \}$ such that $\frac{N_1}{t_1} = \frac{N_2}{t_2} = ... = \frac{N_s}{t_s}$ and $\frac{N_{s+1}}{t_{s+1}} = \frac{N_{s+2}}{t_{s+2}} = ... = \frac{N_n}{t_n}$, then $\mu_n = -\mu_1 = -\sqrt{\frac{\sum_{i=1}^{n} N_i^2}{\sum_{i=1}^{n} t_i^2}}$. From again $\sum_{i=1}^{n} \mu_i^2 = 2|E(T)| = 2(n-1)$, we have that $\mu_i = \sqrt{\frac{2(n-1-\mu_1^2)}{n-2}}$, where $2 \leq i \leq r$, and $\mu_j = -\sqrt{\frac{2(n-1-\mu_1^2)}{n-2}}$, where

$r+1 \leq j \leq n-2$. QED

Note that Yu, Lu, and Tian proved the following theorem in [6]

Theorem 5. [6] Let G be a connected bipartite graph of order n. Then

$$\mu_1 \geq \sqrt{\frac{\sum_{i=1}^n (d_i^2 + t_i)}{\sum_{i=1}^n d_i^2}},$$

where the equality holds if and only if G is a semiregular connected bipartite graph.

They in [6] also proved that

$$\sqrt{\frac{\sum_{i=1}^n (d_i^2 + t_i)}{\sum_{i=1}^n d_i^2}} \geq 2\sqrt{\frac{\sum_{i=1}^n d_i^2}{n}} \geq 2\sqrt{\frac{(\sum_{i=1}^n d_i)^2}{n^2}} \geq \frac{4|E(G)|}{n}.$$

Thus, for any tree T of order $n \geq 3$, we have that

$$\sqrt{\frac{\sum_{i=1}^n (d_i^2 + t_i)}{\sum_{i=1}^n d_i^2}} \geq \frac{4|E(T)|}{n} = \frac{4(n-1)}{n} \geq \sqrt{\frac{2(n-1)}{n}}.$$

Notice that

$$\sqrt{\frac{3n-4}{2}} \geq \sqrt{n-1} \geq \mu_1 \geq \sqrt{\frac{\sum_{i=1}^n (d_i^2 + t_i)}{\sum_{i=1}^n d_i^2}}.$$

Hence, we can prove the following theorem via using a very similar argument as the one in the proof of Theorem 1.

Theorem 6. Let T be a tree of $n \geq 3$ vertices and let $f(x)$ be $(1+x^2)^2(3n-4-2x^2)^{n-2}$. Then

$$Z(T) \leq \sqrt{\frac{f\left(\sqrt{\frac{\sum_{i=1}^n (d_i^2+t_i)}{\sum_{i=1}^n d_i^2}}\right)}{(n-2)^{(n-2)}}}.$$

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