MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **78** (2017) 405-416

ISSN 0340 - 6253

On Harmonic Index of Trees

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(Received March 15, 2016)

Abstract

The Harmonic index of a graph G, denoted by $H(G)$, is defined as the sum of terms $2/[d(u)+d(v)]$ over all edges uv of G, where $d(u)$ denotes the degree of a vertex u. Zhong [L. Zhong, *Appl. Math. Lett.* **25** (2012) 561–566] proved that for any tree T of order $n \geq 5$, $H(T) \leq \frac{4}{3} + \frac{n-3}{2}$. We generalize this result and show that for any tree T of order $n \geq 5$ with maximum degree Δ,

$$H(T) \leqslant \begin{cases} 2\left(\frac{2\Delta-n+1}{\Delta+1} + \frac{n-\Delta-1}{\Delta+2} + \frac{n-\Delta-1}{3}\right) & \text{if } \Delta > \frac{n-1}{2} \\ 2\left(\frac{\Delta}{\Delta+2} + \frac{\Delta}{3} + \frac{n-2\Delta-1}{4}\right) & \text{if } \Delta \leq \frac{n-1}{2} \end{cases}$$

and characterize the extremal trees. Moreover, we obtain a lower bound for $H(T)$.

1 Introduction

Let G be a simple connected graph with vertex set $V = V(G)$ and edge set $E = E(G)$. The order $|V|$ of G is denoted by $n = n(G)$ and the size $|E|$ of G is denoted by $m = m(G)$. For every vertex $v \in V$, its *open neighborhood* $N(v)$ is the set

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$\{u \in V(G) \mid uv \in E(G)\}$. The *degree* of a vertex $v \in V$ is $d(v) = |N(v)|$. The minimum and maximum degree of a graph G are denoted by $\delta = \delta(G)$ and $\Delta = \Delta(G)$, respectively. A *leaf* of a tree T is a vertex of degree 1, a *stem* is a vertex adjacent to a leaf, whereas and a *strong stem* is a stem adjacent to at least two leaves. An *end stem* is a stem whose all neighbors with exception at most one are leaves.

A *rooted tree* is a directed tree having a distinguished vertex ω, called the *root*.

A large variety of degree–based topological indices has been defined in the mathematical and mathematico–chemical literature; for details see [4, 5]. Here, we are concerned with the *harmonic index*.

For a simple graph $G = (V, E)$, the harmonic index of G, denoted $H(G)$, is defined in [2] as the sum of terms $2/[d(u) + d(v)]$ over all edges uv of the underlying graph. That is,

$$H = H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)} .$$

In [10, 26–29, 33], the minimum and maximum harmonic indices of simple connected graphs, trees, unicyclic, and bicyclic graphs were determined and the corresponding extremal graphs characterized. For other related works see [19, 34–36]. Wu et al. [23] established a lower bound on H of a graph with minimum degree two. Favaron et al. [3] investigated the relation between graph eigenvalues of graphs and H. Deng et al. [1] considered the relation between $H(G)$ and the chromatic index $\chi(G)$, and proved that $\chi(G) \leq 2H(G)$. Liu [14] proposed a conjecture concerning the relation between the harmonic index and the diameter of a connected graph, and showed that the conjecture is true for trees. Relationships between the harmonic index and several other topological indices were established in [8, 11, 25, 31]. For additional results on this index, see [12, 13, 15–18, 21, 24, 30].

Zhong [26] proved the following upper bound on the harmonic index of trees.

Theorem A. *For any tree T of order $n \geq 5$,*

$$H(T) \leq \frac{4}{3} + \frac{n-3}{2}$$

with equality if and only if $T \cong P_n$.

In this paper, as a generalization of the aforementioned result, we establish a best possible upper bound for the harmonic index of trees in terms of their order and maximum degree and characterize all extreme trees. We also present a lower bound for the harmonic index of trees.

2 An upper bound on the harmonic index of trees

In this section we present a sharp upper bound for the harmonic index of trees in terms of their order and maximum degree, and characterize all extreme trees. Throughout this section, T denote a rooted tree with root ω where ω is a vertex of maximum degree and $N(\omega) = \{w_1, w_2, \ldots, w_\Delta\}$. In addition, $h_\omega : E(T) \to \mathbb{R}$ is a function defined by $h_\omega(uv) = 1/[d(u) + d(v)]$. Hence $H(T) = \sum_{e \in E(T)} h_\omega(e)$.

We start with some lemmas.

Lemma 1. *Let T be a tree of order n with maximum degree Δ. If T has an end-stem of degree at least three, different from ω, then there is a tree T' of order n with maximum degree Δ, such that $H(T) < H(T')$.*

Proof. Let $v \neq \omega$ be an end-stem of T with $d(v) = \beta \geqslant 3$ and let $N(v) = \{v_1, v_2, \ldots, v_{\beta-1}, u\}$ where u is the parent of v. Assume that $d(u) = t$. Let $S = \{vv_1, vv_2, \ldots, vv_{\beta-2}, vv_{\beta-1}, vu\}$ and let T' be the tree obtained from $T \setminus \{v_1, \ldots, v_{\beta-2}\}$ by attaching the path $v_{\beta-1}v_{\beta-2} \ldots v_3v_2v_1$ (see Figure 1). Clearly, T' is a tree of order n with $\Delta(T) = \Delta(T')$. By definition, we have

$$\frac{1}{2}H(T) = \sum_{uv \notin S} h_\omega(uv) + \sum_{uv \in S} h_\omega(uv) = \sum_{uv \notin S} h_\omega(uv) + \frac{1}{\beta + t} + \frac{\beta - 2}{\beta + 1} + \frac{1}{\beta + 1} \qquad (1)$$

and

$$\frac{1}{2}H(T') = \sum_{uv \notin S} h_\omega(uv) + \frac{1}{2 + t} + \frac{\beta - 2}{4} + \frac{1}{3}\,. \qquad (2)$$

Combining (1) and (2) and using the fact that $\beta \geq 3$, we get $H(T) < H(T')$, as desired. $\square$

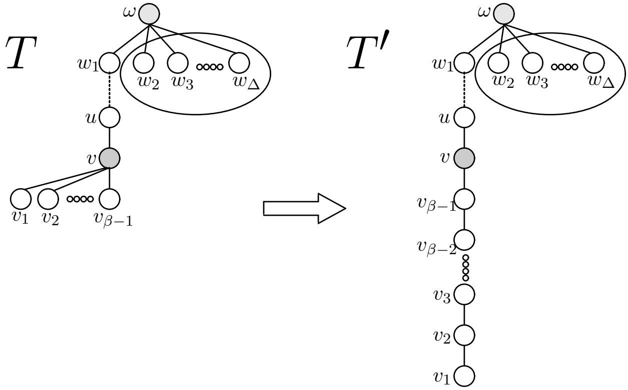


Figure 1: The trees T and T' used in the proof of Lemma 1.

Lemma 2. *Let T be a tree of order n with maximum degree Δ. If T has a stem of degree at least three, different from ω, then there is a tree T' of order n with maximum degree Δ such that $H(T) < H(T')$.*

Proof. Let $u \neq \omega$ be a stem of T of degree $d(v) = \beta \geq 3$ and let $N(u) = \{u_1, u_2, \cdots, u_{\beta-1}, v\}$ where $d(v) = 1$ and u_1 is the parent of u. By Lemma 1, we may assume that u is not an end-stem. Suppose that T_i is the component of $T \setminus \omega$ containing w_i. Further, let $p_i \in V(T_i)$ be a leaf with maximum distance from w_i, and z be its parent (see Figure 2). Then $d(z) = 2$ by Lemma 1.

Let T' be the tree obtained from $T \setminus uv$ by adding a pendent edge $p_i v$ (see Figure 2) and let $S = \{p_i z, uv, uu_1, uu_2, \ldots, uu_{\beta-1}\}$. Clearly, T' is a tree of order n with $\Delta(T) = \Delta(T')$. Now we show that $H(T) < H(T')$. By definition we have

$$\frac{1}{2}H(T) = \sum_{uv \notin S} h_\omega(uv) + \sum_{uv \in S} h_\omega(uv) = \sum_{uv \notin S} h_\omega(uv) + \frac{1}{\beta+1} + \sum_{i=1}^{\beta-1} \frac{1}{d_{u_i} + \beta} + \frac{1}{3} \quad (3)$$

and

$$\frac{1}{2}H(T') = \sum_{uv \notin S} h_\omega(uv) + \frac{1}{4} + \sum_{i=1}^{\beta-1} \frac{1}{d_{u_i} + \beta - 1} + \frac{1}{3}. \quad (4)$$

Applying (3) and (4), we conclude that $H(T) < H(T')$ and the proof is complete. □

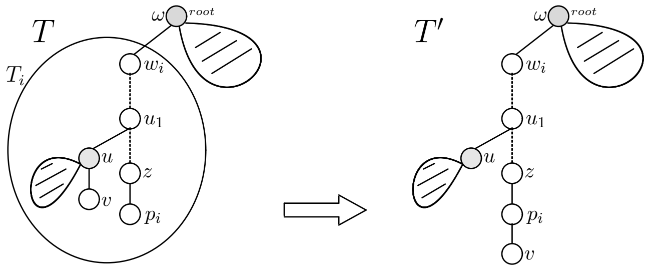


Figure 2: The trees T and T' used in the proof of Lemma 2.

Lemma 3. *Let T be a tree of order n with maximum degree Δ. If T has a vertex of degree at least three, different from ω, then there is a tree T' of order n with maximum degree Δ such that $H(T) < H(T')$.*

Proof. Let $v \neq \omega$ be a vertex of degree $d(v) = \beta \geq 3$ such that $d(\omega, v)$ is as large as possible and let $N(v) = \{u_1^0, u_2^0, \ldots, u_{\beta-1}^0, u_\beta\}$ where u_β is the parent of v. Let $u_i^0 u_i^1 \ldots u_i^{t_i}$ be the longest path in T_i beginning at u_i^0 for $i = 1, \ldots, \beta - 1$. Assume that $p_i \in V(T_i)$ is a leaf with maximum distance from w_i and let z be the parent of p_i (see Figure 3). We may assume that $p_i \notin \{u_1^{t_1}, \ldots, u_{\beta-2}^{t_{\beta-2}}\}$. By Lemmas 1 and 2, and the choice of v, we may assume that $d(z) = 2$ and that all descendants of v with exception of leaves, have degree two. Consider two cases.

Case 1. $\beta = 3$.

Let T' be the tree obtained from $T \setminus vu_1^0$ by adding the edge $p_i u_1^0$ (see Figure 3). Evidently, T' is a tree of order n with $\Delta(T') = \Delta(T)$. Let $S = \{vu_1^0, vu_2^0, vu_3, p_i z\}$. By definition, we have

$$\frac{1}{2}H(T) = \sum_{uv \notin S} h_\omega(uv) + \sum_{uv \in S} h_\omega(uv) = \sum_{uv \notin S} h_\omega(uv) + \frac{1}{5} + \frac{1}{5} + \frac{1}{3 + d_{u_3}} + \frac{1}{3}$$

and

$$\frac{1}{2}H(T') = \sum_{uv \notin S} h_\omega(uv) + \frac{1}{4} + \frac{1}{4} + \frac{1}{2 + d_{u_3}} + \frac{1}{4}.$$

Clearly, $H(T) < H(T')$ and we are done.

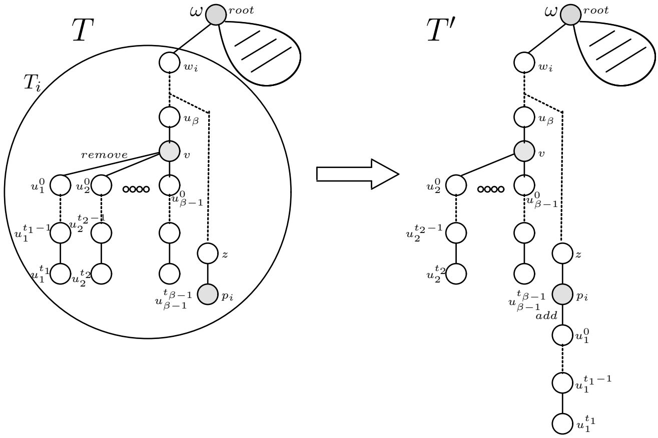


Figure 3: The trees T and T' used in the proof of Lemma 3.

Case 2. $\beta \geq 4$.

First let $p_i \neq u_{\beta-1}^{t_{\beta-1}}$. Let T' be the tree obtained from T be deleting the edges $u_1^0 v, u_2^0 v, \ldots, u_{\beta-1}^0 v$ and adding new edges $u_1^0 p_i, u_2^0 u_1^{t_1}, u_3^0 u_2^{t_2}, \ldots, u_{\beta-1}^0 u_{\beta-2}^{t_{\beta-2}}$. Obviously, T' is a tree of order n with $\Delta(T') = \Delta(T)$. Assume that

$$S = \{p_i z, v u_\beta\} \cup \{v u_i^0, u_i^{t_i} u_i^{t_i - 1} \mid 1 \leq i \leq \beta - 1\}.$$

By definition, we have

$$\frac{1}{2}H(T) = \sum_{uv \notin S} h_\omega(uv) + \sum_{uv \in S} h_\omega(uv) = \sum_{uv \notin S} h_\omega(uv) + \frac{\beta-1}{3} + \frac{1}{3} + \frac{\beta-1}{\beta+2} + \frac{1}{\beta + d_{u_\beta}}$$

and

$$\frac{1}{2}H(T') = \sum_{uv \notin S} h_\omega(uv) + \frac{\beta-1}{4} + \frac{1}{3} + \frac{\beta-1}{4} + \frac{1}{1 + d_{u_\beta}}.$$

It is easy to verify that $H(T) < H(T')$.

Now let $p_i = u_{\beta-1}^{t_{\beta-1}}$. Let T' be the tree obtained from T by deleting the edges $v u_i^0$ for $i = 1, \ldots, \beta - 2$ and by adding the edges $u_1^0 p_i$, $u_i^{t_i} u_{i+1}^0$ for $1 \leq i \leq \beta - 3$. Suppose that $S = \{v u_\beta\} \cup \{v u_i^0, u_i^{t_i} u_i^{t_i-1} \mid 1 \leq i \leq \beta - 1\}$. It follows from definition that

$$\frac{1}{2}H(T) = \sum_{uv \notin S} h_\omega(uv) + \sum_{uv \in S} h_\omega(uv) = \sum_{uv \notin S} h_\omega(uv) + \frac{\beta-1}{3} + \frac{\beta-1}{\beta+2} + \frac{1}{\beta + d_{u_\beta}} \quad (5)$$

and

$$\frac{1}{2}H(T') = \sum_{uv \notin S} h_\omega(uv) + \frac{\beta-2}{4} + \frac{1}{3} + \frac{\beta-1}{4} + \frac{1}{2+d_{u_\beta}}\,. \tag{6}$$

Since

$$\frac{1}{\beta+d_{u_\beta}} < \frac{1}{2+d_{u_\beta}} \qquad , \qquad \frac{\beta-1}{3} + \frac{\beta-1}{\beta+2} \leqslant \frac{\beta-1}{2}$$

and

$$\frac{\beta-2}{4} + \frac{1}{3} + \frac{\beta-1}{4} = \frac{\beta-1}{2} + \frac{1}{12}$$

we conclude from (5) and (6) that $H(T') > H(T)$ and the proof is complete. □

A spider (or a starlike tree [20, 22]) is a tree with at most one vertex of degree greater than 2. The vertex of degree greater than two is called the center of the spider. (If there are no vertices of degree greater than two, then any vertex can be the center.) A leg of a spider is a path from the center to a vertex of degree 1. Thus, a star with k edges is a spider of k legs, each of length 1, whereas the path is a spider with one or two legs.

Lemma 4. *Let T be a spider of order n with $k \geq 3$ legs. If T has a leg of length 1 and a leg of length greater than 2, then there is a spider T' of order n with k legs such that $H(T) < H(T')$.*

Proof. Let ω be the center of T and $N(\omega) = \{w_1, \ldots, w_k\}$. Let the root of T be at ω. Without loss of generality assume that $d(w_1) = 1$ and let $w_k x_1 x_2 \ldots x_t$ be a longest leg of T. Let T' be the tree obtained from T by deleting the edge $x_t x_{t-1}$ and adding the pendent edge $w_1 x_t$. Suppose that $S = \{w_1\omega, x_t x_{t-1}, x_{t-2}x_{t-1}\}$. By definition, we have

$$\frac{1}{2}H(T) = \sum_{uv \notin S} h_\omega(uv) + \sum_{uv \in S} h_\omega(uv) = \sum_{uv \notin S} h_\omega(uv) + \frac{1}{k+1} + \frac{1}{3} + \frac{1}{4} \tag{7}$$

and

$$\frac{1}{2}H(T') = \sum_{uv \notin S} h_\omega(uv) + \frac{1}{k+2} + \frac{1}{3} + \frac{1}{3}\,. \tag{8}$$

It is easy to see that $H(T') > H(T)$ as desired. □

Now we are ready to state our mail result.

Theorem 5. *For any tree T of order $n \geq 5$ with maximum degree Δ,*

$$H(T) \leqslant \begin{cases} 2\left(\frac{2\Delta-n+1}{\Delta+1} + \frac{n-\Delta-1}{\Delta+2} + \frac{n-\Delta-1}{3}\right) & \text{if } \Delta > \frac{n-1}{2} \\ 2\left(\frac{\Delta}{\Delta+2} + \frac{\Delta}{3} + \frac{n-2\Delta-1}{4}\right) & \text{if } \Delta \leq \frac{n-1}{2} \end{cases}$$

with equality if and only if T is a spider whose all legs have length at most two or all legs have length at least two.

Proof. Let T_1 be a tree of order $n \geq 5$ with maximum degree Δ such that

$$H(T_1) = \max\{H(T) \mid T \text{ is a tree of order } n \text{ with maximum degree } \Delta\}.$$

Let ω be a vertex with maximum degree Δ and let the root of T_1 be at ω. If $\Delta = 2$, then T is a path of order n and the result follows by Theorem A.

Let therefore $\Delta \geq 3$. By the choice of T_1, we deduce from Lemmas 1, 2, and 3 that T_1 is a spider with center ω. It follows from Lemma 4 and the choice of T_1 that all legs of T_1 either have length at most two or have length at least two.

First, let all legs of T_1 be of length at least two. Then clearly $\Delta \leq \frac{n-1}{2}$ and

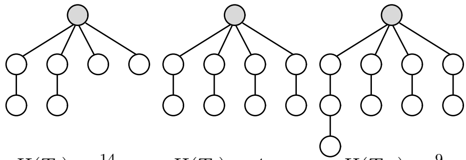
$$H(T_1) = 2\left(\frac{\Delta}{\Delta+2} + \frac{\Delta}{3} + \frac{n-2\Delta-1}{2}\right)$$

as desired. Now let all legs of T_1 be of length at most two. Bearing in mind the above case, we may assume that T_1 has a leg of length 1. If T_1 is a star, then the result is immediate. Assume that T_1 is not a star. Then the number of leaves adjacent to ω is $2\Delta + 1 - n$ and hence

$$H(T) = 2\left(\frac{2\Delta - n + 1}{\Delta + 1} + \frac{n - \Delta - 1}{\Delta + 2} + \frac{n - \Delta - 1}{3}\right).$$

This completes the proof. □

In Figure 4 are depicted three trees of orders $n = 7, 9, 10$ with maximum degree $\Delta = 4$ and with maximum harmonic index.



$H(T_7) = \frac{14}{5}$ $H(T_9) = 4$ $H(T_{10}) = \frac{9}{2}$

Figure 4: Some trees with maximum degree 4 and maximum harmonic index.

3 A lower bound on the harmonic index of trees

In this section we present a lower bound for the harmonic index of trees. Recall that the first Zagreb index of a graph G, denoted by $M_1 = M_1(G)$, is equal to the sum of squares of the degrees of the vertices. That is,

$$M_1(G) = \sum_{u \in V(G)} d(u)^2 = \sum_{uv \in E(G)} \big[d(u) + d(v)\big] .$$

For details on M_1 we refer the readers to [5–7]. In [9, 32], the following result was proven:

Theorem B. *Let T be a tree of order n and maximum degree Δ. Then*

$$M_1(T) \leq \begin{cases} (\Delta+2)n - 4\Delta + 4 & \text{if } r = 0 \\ (\Delta+2)n - 3\Delta & \text{if } r = 1 \\ (\Delta+2)n - 2\Delta - 2 & \text{if } r = 2 \\ (\Delta+2)n - 2\Delta - 3 + r(r-2) & \text{if } r \geq 3 \end{cases}$$

where $n \equiv r$ (mod $\Delta - 1$).

Xu in [25], proved that for any connected graph G of order n and size m,

$$H(G) \geqslant \frac{2m^2}{M_1(G)} .$$

The next result is an immediate consequence of Theorem B and the above inequality, where we take into account that for trees, $m = n - 1$.

Corollary 6. *Let T be a tree of order n and $n \equiv r$ (mod $\Delta - 1$). Let Δ be the maximum degree of T. Then*

$$H(T) \geqslant \begin{cases} \dfrac{2(n-1)^2}{(\Delta+2)n - 4\Delta + 4} & \text{if } r = 0 \\[2ex] \dfrac{2(n-1)^2}{(\Delta+2)n - 3\Delta} & \text{if } r = 1 \\[2ex] \dfrac{2(n-1)^2}{(\Delta+2)n - 2\Delta - 2} & \text{if } r = 2 \\[2ex] \dfrac{2(n-1)^2}{(\Delta+2)n - 2\Delta - 3 + r(r-2)} & \text{if } r \geq 3\,. \end{cases}$$

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