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The harmonic index for graphs

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ABSTRACT

The harmonic index of a graph G is defined as the sum of the weights $\frac{2}{d(u)+d(v)}$ of all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G. In this work, we present the minimum and maximum values of the harmonic index for simple connected graphs and trees, and characterize the corresponding extremal graphs.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The Randić index $R(G)$, proposed by Randić [1] in 1975, is defined as the sum of the weights $(d(u)d(v))^{-\frac{1}{2}}$ over all edges uv of G, that is,

$$R(G) = \sum_{uv\in E(G)} (d(u)d(v))^{-\frac{1}{2}},$$

where $d(u)$ denotes the degree of a vertex u of G. The Randić index is one of the most successful molecular descriptors in structure–property and structure–activity relationship studies [2–5]. Mathematical properties of this descriptor have also been studied extensively, as summarized in [6,7].

With motivation from the Randić index, the sum-connectivity index $\chi(G)$ and the general sum-connectivity index $\chi_\alpha(G)$ were recently proposed by Zhou and Trinajstić in [8,9] and defined as

$$\chi(G) = \sum_{uv\in E(G)} (d(u)+d(v))^{-\frac{1}{2}}$$

and

$$\chi_\alpha(G) = \sum_{uv\in E(G)} (d(u)+d(v))^{\alpha},$$

where α is a real number. It has been found that the (general) sum-connectivity index and the Randić index correlate well between themselves and with the π-electronic energy of benzenoid hydrocarbons [10,11]. Some mathematical properties of the (general) sum-connectivity index on trees, molecular trees, unicyclic graphs and bicyclic graphs were given in [8,9,12–16].

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In this work, we consider another variant of the Randić index, named the harmonic index. For a graph G, the harmonic index $H(G)$ is defined as

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

As far as we know, this index first appeared in [17]. Favaron et al. [18] considered the relation between the harmonic index and the eigenvalues of graphs. Here we will consider the minimum and maximum values of the harmonic index for simple connected graphs and trees, and characterize the corresponding extremal graphs.

It is easy to see that for any graph G, we always have $H(G) = 2\chi_{-1}(G)$ and $H(G) \le R(G)$ with equality if and only if G is a regular graph. Since the regular graphs have the maximum value $\frac{n}{2}$ of the Randić index among all the graphs with n vertices [19], we deduce that the regular graphs are also the extremal graphs with the maximum value of the harmonic index.

We conclude this section with some notation and terminology. Let G be a graph. For any vertex $v \in V(G)$, we use $N_G(u)$ (or $N(u)$ if there is no ambiguity) to denote the set of neighbors of v in G. We denote by $\delta(G)$ the minimum degree of G. We define $G - uv$ to be the graph obtained from G by deleting the edge $uv \in E(G)$, and $G + uv$ to be the graph that arises from G by adding an edge uv between two non-adjacent vertices u and v of G. We use S_n and P_n to denote the star and the path on n vertices, respectively.

We write $A := B$ to rename B as A. For any graph G and for two distinct vertices u and v of G, the distance between u and v in G is the number of edges in a shortest path joining u and v. The diameter of G is the maximum distance between any two vertices of G. Let T be a tree with diameter k; then a main chain of T is a path of length k in T. Clearly, if P^* is a main chain of T, then the two endvertices of P^* have degree exactly 1 in T.

2. The minimum value of the harmonic index for trees

In this section, we consider the minimum value of the harmonic index for trees with n vertices, and we show that the extremal graph is S_n.

Theorem 1. *Let T be a tree of order $n \ge 3$; then $H(T) \ge \frac{2(n-1)}{n}$ with equality if and only if $T \cong S_n$.*

Proof. Since $S_3 = P_3$ is the unique tree with three vertices, it is easy to check that Theorem 1 is true for $n = 3$. Suppose the theorem holds for $n = k \ge 3$; we next show that it also holds for $n = k + 1$.

Let T be a tree of order $k + 1$. Then T contains at least two leaves. Let uv be an edge in T with $d(v) = 1$. Since $k \ge 3$, we have $2 \le d(u) = d \le k$. Let $N(u) \setminus \{v\} = \{v_1, v_2, \ldots, v_{d-1}\}$ with $d(v_i) = p_i$ for each $1 \le i \le d - 1$, and let $T' := T - \{v\}$. Then T' is a tree with k vertices. By the induction hypothesis, we have $H(T') \ge \frac{2(k-1)}{k}$. Hence

$$\begin{aligned}
H(T) &= H(T') + \frac{2}{d+1} + \sum_{i=1}^{d-1} \frac{2}{p_i + d} - \sum_{i=1}^{d-1} \frac{2}{p_i + d - 1} \\
&= H(T') + \frac{2}{d+1} - \sum_{i=1}^{d-1} \frac{2}{(p_i + d - 1)(p_i + d)} \ge \frac{2(k-1)}{k} + \frac{2}{d+1} - \sum_{i=1}^{d-1} \frac{2}{d(d+1)} \\
&= \frac{2(k-1)}{k} + \frac{2}{d(d+1)} \ge \frac{2(k-1)}{k} + \frac{2}{k(k+1)} = \frac{2k}{k+1},
\end{aligned}$$

and the equality holds if and only if $T \cong S_{k+1}$. This completes the proof of Theorem 1. □

3. The maximum value of the harmonic index for trees

The aim of this section is to show that P_n has the maximum value of the harmonic index among all the trees with n vertices. Since $P_3 = S_3$ is the unique tree with three vertices, we only consider $n \ge 4$ in the following.

First, we prove the following two lemmas.

Lemma 1. *Let T^* be a tree of order $n \ge 4$ with the maximum value of the harmonic index, and let $P^* = u_0u_1u_2 \ldots u_d$ be a main chain of T^*; then $d(u_1) = 2$.*

Proof. Since $n \ge 4$, we know that $d \ge 3$; for otherwise, $T^* \cong S_n$ has the minimum value of the harmonic index by Theorem 1, a contradiction. By the definition of the main chain, we have $d(u_0) = d(u_d) = 1$ and $d(u_i) \ge 2$ for $1 \le i \le d - 1$.

Suppose to the contrary that $d(u_1) = x \ge 3$. Let $N(u_1) \setminus \{u_0, u_2\} = \{v_1, v_2, \ldots, v_{x-2}\}$, and let $d(u_2) = y \ge 2$. Then $d(v_i) = 1$ for each $1 \le i \le x - 2$; otherwise, it is easy to see that there exists a path of length at least $d + 1$ in T^*, a contradiction.

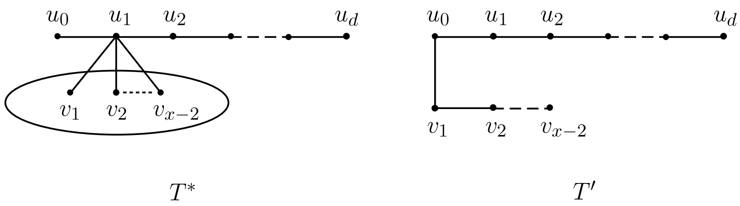

Fig. 3.1. T^* and T'.

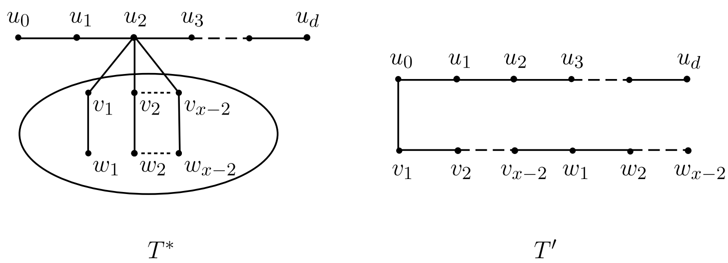

Fig. 3.2. T^* and T'.

Let $T' := T^* - \{u_1v_1, u_1v_2, \ldots, u_1v_{x-2}\} + \{u_0v_1, v_1v_2, \ldots, v_{x-3}v_{x-2}\}$; see Fig. 3.1. Then T' is a tree with diameter at least $d+1$, and hence $T' \ncong T^*$. Therefore

$$\begin{aligned} H(T') - H(T^*) &= \frac{2}{3} + \frac{x-2}{2} + \frac{2}{y+2} - \frac{2(x-1)}{x+1} - \frac{2}{x+y} \\ &= \frac{3x^2 - 11x + 10}{6(x+1)} + \frac{2(x-2)}{(y+2)(x+y)} > 0, \end{aligned}$$

and the last inequality holds since $x \geq 3$. But this implies that $H(T') > H(T^*)$, which contradicts the choice of T^*. So Lemma 1 holds. □

Lemma 2. *Let T^* be a tree of order $n \geq 4$ with the maximum value of the harmonic index, and let $P^* = u_0u_1u_2 \ldots u_d$ be a main chain of T^*; then $d(u_2) = 2$.*

Proof. By the argument in Lemma 1, we deduce that $d \geq 3$, $d(u_1) = 2$ and $d(u_i) \geq 2$ for each $2 \leq i \leq d-1$.

Suppose for a contradiction that $d(u_2) = x \geq 3$. Let $N(u_2) \setminus \{u_1, u_3\} = \{v_1, v_2, \ldots, v_{x-2}\}$, and let $d(u_3) = y$. If there exists some v_i $(1 \leq i \leq x-2)$ such that $d(v_i) = 1$, then let $T_1 := T^* - u_2v_i + u_0v_i$, and it is easy to check that $H(T_1) > H(T^*)$, a contradiction. So we may assume that $d(v_i) \geq 2$ for each $1 \leq i \leq x-2$.

Let $N(v_1) \setminus \{u_2\} = \{w_1, w_2, \ldots, w_k\}$. Then we have $d(w_j) = 1$ for each $1 \leq j \leq k$; for otherwise, we can easily find a path of length at least $d+1$ in T^*, a contradiction. If $k \geq 2$, then let $T_2 := T^* - v_1w_1 + u_0w_1$, and it is easy to calculate that $H(T_2) > H(T^*)$, again a contradiction. Therefore we may further assume that $k = 1$, and hence $d(v_1) = 2$.

By the same argument as for v_1, we can conclude that for each $1 \leq i \leq x-2$, $d(v_i) = 2$ and $d(w_i) = 1$, where $w_i = N(v_i) \setminus \{u_2\}$.

Now let $T' := T^* - \{u_2v_1, v_1w_1, u_2v_2, v_2w_2, \ldots, u_2v_{x-2}, v_{x-2}w_{x-2}\} + \{u_0v_1, v_1v_2, \ldots, v_{x-2}w_1, w_1w_2, \ldots, w_{x-3}w_{x-2}\}$; see Fig. 3.2. Then T' is a tree with diameter at least $d+2$, and hence $T' \ncong T^*$. Therefore

$$\begin{aligned} H(T') - H(T^*) &= x - 2 + \frac{1}{2} + \frac{2}{y+2} - \frac{2(x-1)}{x+2} - \frac{2}{x+y} - \frac{2(x-2)}{3} \\ &= \frac{2x^2 - 9x + 10}{6(x+2)} + \frac{2(x-2)}{(y+2)(x+y)} > 0, \end{aligned}$$

and the last inequality holds since $x \geq 3$. But now we have $H(T') > H(T^*)$, contradicting the choice of T^*. This proves Lemma 2. □

We can now prove the main result of this section.

Theorem 2. *Let T be a tree of order $n \geq 4$; then $H(T) \leq \frac{4}{3} + \frac{n-3}{2}$ with equality if and only if $T \cong P_n$.*

Proof. Since P_4 and S_4 are the only two trees with four vertices, it is easy to calculate that $H(P_4) = \frac{4}{3} + \frac{1}{2} > \frac{3}{2} = H(S_4)$. This implies that Theorem 2 is true for $n = 4$. Suppose the theorem holds for $n = k \geq 4$; we now show that it also holds for $n = k+1$.

Let T^* be a tree of order $k+1$ with the maximum value of the harmonic index, and let $P^* = u_0 u_1 \dots u_d$ be a main chain of T^*. Then by Lemmas 1 and 2, we know that $d(u_1) = d(u_2) = 2$. Let $T' := T^* - \{u_0\}$. Then T' is a tree with k vertices. By the induction hypothesis, we have $H(T') \leq \frac{4}{3} + \frac{k-3}{2}$. Then

$$H(T^*) = H(T') + \frac{1}{2} \leq \frac{4}{3} + \frac{k-3}{2} + \frac{1}{2} = \frac{4}{3} + \frac{(k+1)-3}{2}$$

with equality if and only if $T^* \cong P_{k+1}$. This completes the proof of the theorem. □

4. The minimum value of the harmonic index for general graphs

In this section, we consider the minimum value of the harmonic index for simple connected graphs of order n, and we show that the extremal graph is still S_n. It follows from the proof of Theorem 1 that we need only show that any extremal graph with the minimum value of the harmonic index must have some vertex of degree 1. For this purpose, we prove the following two lemmas.

Lemma 3. *Let G^* be a simple connected graph of order $n \geq 4$ with the minimum value of the harmonic index; then there exists an edge in G^* which is not contained in any triangle.*

Proof. Suppose to the contrary that every edge of G^* is contained in some triangle. Then $\delta(G^*) \geq 2$. We consider three cases according to the value of $\delta(G^*)$.

Case 1. $\delta(G^*) = 2$.

Let w be a vertex of degree 2 in G^* with $N(w) = \{u, v\}$. Then $uv \in E(G^*)$. By the symmetry between u and v, we may assume that $k = d(v) \leq d(u) = l$. Let $G' := G^* - vw$.

If $k = 2$, then

$$H(G') - H(G^*) = \frac{4}{l+1} - \frac{4}{l+2} - \frac{1}{2} = \frac{4}{(l+1)(l+2)} - \frac{1}{2} \leq \frac{4}{3 \times 4} - \frac{1}{2} < 0,$$

a contradiction. So we may assume that $k \geq 3$.

Let $N(v) \setminus \{w, u\} = \{v_1, v_2, \dots, v_{k-2}\}$ with $d(v_i) = p_i$. Then $p_i \geq 2$ for each $1 \leq i \leq k-2$. Hence

$$\begin{aligned} H(G') - H(G^*) &= \sum_{i=1}^{k-2} \frac{2}{p_i + k - 1} + \frac{2}{l+1} + \frac{2}{l+k-1} - \sum_{i=1}^{k-2} \frac{2}{p_i + k} - \frac{2}{l+2} - \frac{2}{k+2} - \frac{2}{l+k} \\ &= \sum_{i=1}^{k-2} \frac{2}{(p_i + k - 1)(p_i + k)} + \frac{2}{(l+k-1)(l+k)} + \frac{2}{(l+1)(l+2)} - \frac{2}{k+2} \\ &\leq \frac{2(k-2)}{(k+1)(k+2)} + \frac{2}{(k+1)(k+2)} + \frac{2}{(k+1)(k+2)} - \frac{2}{k+2} = -\frac{2}{(k+1)(k+2)} < 0, \end{aligned}$$

again a contradiction.

Case 2. $\delta(G^*) = 3$.

Let w be a vertex of degree 3 in G^* with $N(w) = \{v_1, v_2, v_3\}$. Since every edge of G^* is contained in some triangle, there exist at least two edges among the vertices v_1, v_2 and v_3. Without loss of generality, we may assume that $v_1v_2, v_2v_3 \in E(G^*)$. By the symmetry between v_1 and v_3, let $x = d(v_1) \leq d(v_3) = z$ and let $d(v_2) = y$. If $v_1v_3 \in E(G^*)$, we may further assume that $x \leq y \leq z$ (since in this case, v_1, v_2 and v_3 are equivalent).

Suppose that $v_1v_3 \notin E(G^*)$ and $z \leq y$. Then $3 \leq x \leq z \leq y$. Let $G' := G^* - \{wv_1, wv_3\} + v_1v_3$. Therefore

$$\begin{aligned} H(G') - H(G^*) &= \frac{2}{x+z} + \frac{2}{y+1} - \frac{2}{x+3} - \frac{2}{y+3} - \frac{2}{z+3} \\ &= \frac{4}{(y+1)(y+3)} - \frac{2(z-3)}{(x+3)(x+z)} - \frac{2}{z+3} \\ &\leq \frac{4}{(z+1)(z+3)} - \frac{2(z-3)}{(z+3)(z+z)} - \frac{2}{z+3} = \frac{-3z^2 + 4z + 3}{z(z+1)(z+3)} < 0, \end{aligned}$$

a contradiction.

So we may assume that $y \leq z$. Let $x^* = \min\{x, y\}$ and $y^* = \max\{x, y\}$. Then $3 \leq x^* \leq y^* \leq z$. Let $G' := G^* - \{wv_1, wv_2\}$, and let the degree sequences of $N(v_1) \setminus \{w, v_2\}$ and $N(v_2) \setminus \{w, v_1\}$ in G^* be $\{p_1, p_2, \dots, p_{x-2}\}$ and $\{q_1, q_2, \dots, q_{y-2}\}$,

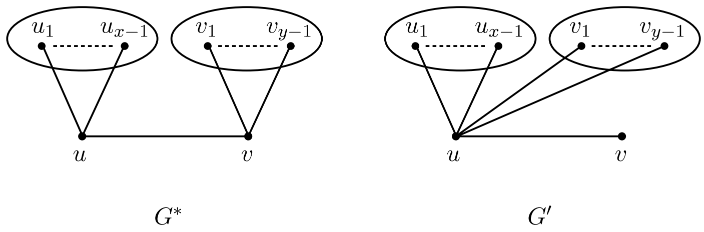

Fig. 4.1. G^* and G'.

respectively. Hence we have

$$\begin{aligned} H(G')-H(G^*) &= \sum_{i=1}^{x-2}\frac{2}{p_i+x-1}+\sum_{j=1}^{y-2}\frac{2}{q_j+y-1}+\frac{2}{z+1}+\frac{2}{x+y-2}-\sum_{i=1}^{x-2}\frac{2}{p_i+x}-\sum_{j=1}^{y-2}\frac{2}{q_j+y}\\ &\quad -\frac{2}{x+3}-\frac{2}{y+3}-\frac{2}{z+3}-\frac{2}{x+y}\\ &= \sum_{i=1}^{x-2}\frac{2}{(p_i+x-1)(p_i+x)}+\sum_{j=1}^{y-2}\frac{2}{(q_j+y-1)(q_j+y)}+\frac{4}{(z+1)(z+3)}\\ &\quad +\frac{4}{(x+y-2)(x+y)}-\frac{2}{x+3}-\frac{2}{y+3}\\ &\le \frac{2(x-2)}{(x+2)(x+3)}+\frac{2(y-2)}{(y+2)(y+3)}+\frac{4}{(y^*+1)(y^*+3)}+\frac{4}{(x^*+x^*-2)(x^*+x^*)}\\ &\quad -\frac{2}{x+3}-\frac{2}{y+3}\\ &= \frac{-7(x^*)^2+13x^*+6}{x^*(x^*-1)(x^*+2)(x^*+3)}+\frac{-4y^*}{(y^*+1)(y^*+2)(y^*+3)}<0, \end{aligned}$$

a contradiction.

Case 3. $\delta(G^*)\ge 4$.

By the Handshaking Lemma, we see that $2m=\sum_{i=1}^{n} d_i\ge 4n$, where $m=|E(G)|$. Then

$$H(G^*)=\sum_{uv\in E(G^*)}\frac{2}{d(u)+d(v)}\ge\frac{2m}{(n-1)+(n-1)}\ge\frac{2\times 2n}{(n-1)+(n-1)}>H(S_n),$$

a contradiction. This completes the proof of Lemma 3. □

Lemma 4. *Let G^* be a simple connected graph of order $n\ge 4$ with the minimum value of the harmonic index; then $\delta(G^*)=1$.*

Proof. Suppose for a contradiction that $\delta(G^*)\ge 2$. By Lemma 3, there exists an edge uv in G^* such that uv is not contained in any triangle. Then $N(u)\cap N(v)=\emptyset$. Let $d(u)=x\ge 2$ and $d(v)=y\ge 2$. Let $N(u)\setminus\{v\}=\{u_1,u_2,\dots,u_{x-1}\}$ with $d(u_i)=p_i$ for each $1\le i\le x-1$, and let $N(v)\setminus\{u\}=\{v_1,v_2,\dots,v_{y-1}\}$ with $d(v_j)=q_j$ for each $1\le j\le y-1$.

Define $G':=G^*-\{vv_1,vv_2,\dots,vv_{y-1}\}+\{uv_1,uv_2,\dots,uv_{y-1}\}$; see Fig. 4.1 for an illustration. Then

$$H(G')-H(G^*)=\sum_{i=1}^{x-1}\frac{2}{p_i+x+y-1}+\sum_{j=1}^{y-1}\frac{2}{q_j+x+y-1}-\sum_{i=1}^{x-1}\frac{2}{p_i+x}-\sum_{j=1}^{y-1}\frac{2}{q_j+y}<0,$$

and the last inequality holds since $x,y\ge 2$. But this shows that $H(G')>H(G^*)$, which contradicts the choice of G^*, and hence the assertion of Lemma 4 holds. □

By Lemma 4 and by the same argument as in the proof of Theorem 1, we have

Theorem 3. *Let G be a simple connected graph of order $n\ge 3$; then $H(G)\ge\frac{2(n-1)}{n}$ with equality if and only if $G\cong S_n$.*

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