On Harmonic Indices of Trees, Unicyclic graphs and Bicyclic graphs

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Abstract

The harmonic index $H(G)$ 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. We determine the $n-$vertex trees with the second and the third for $n \geq 7$, the fourth for $n \geq 10$ and fifth for $n \geq 11$ maximum harmonic indices, and unicyclic graphs with the second and the third for $n \geq 5$, the fourth for $n \geq 7$ and the fifth for $n \geq 8$ maximum harmonic indices, and bicyclic graphs with the maximum for $n \geq 6$, the second and the third for $n \geq 7$ and fourth for $n \geq 9$ maximum harmonic indices.

AMS classification: 05C07, 05C15

Keywords: Harmonic index, Randić index, trees, unicyclic graph, bicyclic graph, pendant path.

1 Introduction

Let $G = (V, E)$ be a simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$. The degree of a vertex v is denoted as d_v. The Randić index is one of the most successful molecular descriptors in structure-property and structure-activity relationships studies. The Randić index $R(G)$ is defined as [1] $R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$.

The mathematical properties of this graph invariant have been studied extensively(see recent book [2] and survey [3]). Motivated by the success of Randić index, various generalizations and modifications were introduced, such as the sum-connectivity [4] and the general sum-connectivity index [5].

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

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}. \tag{1}$$

Let e be the edge of the graph G, connecting the vertices u and v. Then another way of defining $H(G)$ is by associating to the edge e a weight $w(e)$:

$$w(e) = \frac{2}{d_u + d_v}$$

so that the harmonic index is a sum of edge contributions:

$$H(G) = \sum_{edges} w(e). \tag{2}$$

The weight $w(e)$ is positive-valued for all edges e.

In [6] the authors considered the relation between the harmonic index and the eigenvalues of graphs. Zhong in [7, 8] presented the minimum and maximum values of harmonic index on simple connected graphs, trees and unicyclic graphs and characterized the corresponding extremal graphs. Zhong and Xu in [9] studied the harmonic index of bicylic graphs and characterized the corresponding extremal graphs. Deng, Balachandran, Ayyaswamy and Venkatakrishnan in [10] considered the relation relating the harmonic index $H(G)$ and the chromatic number $\chi(G)$ and proved that $\chi(G) \leq 2H(G)$ by using the effect of removal of a minimum degree vertex on the harmonic index. It strengthens a result relating the Randić index and the chromatic number conjectured by the system AutoGraphiX and proved by Hansen et al. in [11]. Deng, Tang and Wu [12] gave a best possible lower bound for the harmonic index of a graph (a triangle-free graph, respectively) with minimum degree at least two and characterize the extremal graphs. Deng, Tang and Zhang [13] considered the harmonic index $H(G)$ and the radius $r(G)$ and strengthened some results relating the Randić index and the radius in [14][15][16]. In this paper, we determine the $n-$vertex trees with the second and the third for $n \geq 7$, the fourth for $n \geq 10$ and fifth for $n \geq 11$ maximum harmonic indices, and unicyclic graphs with the second and the third for $n \geq 5$, the fourth for $n \geq 7$ and the fifth for $n \geq 8$ maximum harmonic indices, and bicyclic graphs with the maximum for $n \geq 6$, the second and the third for $n \geq 7$ and fourth for $n \geq 9$ maximum harmonic indices.

A pendant vertex is a vertex of degree one. A pendant edge is an edge incident with a pendant vertex. A path $u_1u_2...u_r$ in graph G is said to be a pendant path at u_1 if $d_{u_1} \geq 3$, $d_{u_i} = 2$ for $i = 2, ..., r-1$ and $d_{u_r} = 1$, where u_1 is its root.

2 An identity for the harmonic index of a graph

The results outlined in this section apply to arbitrary finite graphs without loops, multiple or directed edges. Let G be such a graph and let n, $n \geq 2$, be the number of its vertices. The greatest possible vertex degree in such a graph is $n-1$.

An edge of G, connecting a vertex of degree i with a vertex of degree j will be called an (i,j) −edge. The number of (i,j) −edges will be denoted by x_{ij}. Clearly, $x_{ij} = x_{ji}$. Eq.(1) can now be rewritten as

$$H(G) = 2 \sum_{1 \leq i \leq j \leq n-1} \frac{x_{ij}}{i+j} \tag{3}$$

Denote by n_i the number of vertices of G, having degree i. Then n_0 is the number of isolated vertices, and

$$n_1 + n_2 + \cdots + n_{n-1} = n - n_0 \tag{4}$$

By counting the edges that end at a vertex of degree i, $i = 1, 2, \cdots, n-1$, one obtains $\sum_{j=1}^{n-1} x_{ij} + x_{ii} = in_i$, i.e.,

$$n_i = \frac{1}{i}\left(\sum_{j=1}^{n-1} x_{ij} + x_{ii}\right) \tag{5}$$

substituting Eq.(5) back into Eq.(4) and performing appropriate rearrangements, we get

$$\sum_{1 \leq i \leq j \leq n-1} \left(\frac{1}{i} + \frac{1}{j}\right) x_{ij} = n - n_0 \tag{6}$$

Now, combining Eqs.(3) and (6), we arrive at

$$n - n_0 - 2H(G) = \sum_{1 \leq i \leq j \leq n-1} \left(\frac{1}{i} + \frac{1}{j} - \frac{4}{i+j}\right) x_{ij}$$

$$= \sum_{1 \leq i \leq j \leq n-1} \left[\frac{(i-j)^2}{(ij)(i+j)}\right] x_{ij}$$

$$H(G) = \frac{n - n_0}{2} - \frac{1}{2} \sum_{1 \le i \le j \le n-1} \left[\frac{(i-j)^2}{(ij)(i+j)} \right] x_{ij} \tag{7}$$

Let, as before, e be the edge of the graph G connecting the vertices u and v. Associate to the edge e a weight $w^*(e)$:

$$w^*(e) = \frac{1}{2} \left[\frac{(d_u - d_v)^2}{(d_u d_v)(d_u + d_v)} \right]$$

Then Eq.(7) is rewritten as

$$H(G) = \frac{n - n_0}{2} - \sum_{edges} w^*(e) \tag{8}$$

For graphs without isolated vertices (in particular, for connected graphs),

$$H(G) = \frac{n}{2} - \sum_{edges} w^*(e) \tag{9}$$

3 Large harmonic indices of trees, unicyclic graphs, and bicyclic graphs

For an $n-$vertex connected graph G, from Eq.(9), we have $H(G) = \frac{n}{2} - \frac{1}{2} f(G)$, where $f(G) = \sum_{uv \in E(G)} \left[\frac{(d_u - d_v)^2}{(d_u d_v)(d_u + d_v)} \right]$. Thus, for a fixed n, $H(G)$ is decreasing on $f(G)$. Using this fact, we will determine trees, unicyclic graphs, and bicyclic graphs with large harmonic indices.

Among the $n-$vertex trees with $n \ge 4$, the path P_n is the unique tree with the maximum harmonic index, which is equal to $\frac{n}{2} - \frac{1}{6}$ (see [7]). Hence, we will determine the $n-$vertex trees with the second for $n \ge 7$, the third for $n \ge 7$, the fourth for $n \ge 10$, the fifth for $n \ge 11$, maximum harmonic indices.

Proposition 1. *Among the $n-$vertex trees,*
(i) For $n \ge 7$, the trees with a single vertex of maximum degree three, adjacent to three vertices of degree two are the trees with the second maximum harmonic index, which is equal to $\frac{n}{2} - \frac{3}{10}$.
(ii) For $n \ge 7$, the trees with a single vertex of maximum degree three, adjacent to one vertex of degree one and two vertices of degree two are the trees with the third maximum harmonic index, which is equal to $\frac{n}{2} - \frac{11}{30}$.
(iii) For $n \ge 10$, the trees with exactly two adjacent vertices of maximum degree three, each adjacent to two vertices of degree two are the trees with the fourth maximum harmonic index, which is equal to $\frac{n}{2} - \frac{2}{5}$.

(iv) For $n \geq 11$, the trees with exactly two vertices of maximum degree three, each adjacent to three vertices of degree two, or the trees with a single vertex of maximum degree three, adjacent to two vertices of degree one and one vertex of degree two are the trees with the fifth maximum harmonic index, which is equal to $\frac{n}{2} - \frac{13}{30}$.

Proof. (i) Let G be an n−vertex tree different from P_n, where $n \geq 4$. Obviously, there are at least three pendant paths in G.

First, the contribution to $f(G)$ of any edge in G is $\frac{(d_u-d_v)^2}{(d_u d_v)(d_u+d_v)} \geq 0$.

Second, note that $\frac{(1-x)^2}{(1)(x)(1+x)}$ and $\frac{(1-2)^2}{(1)(2)(1+2)} + \frac{(2-x)^2}{(2)(x)(2+x)}$ are increasing for $x \geq 3$, a pendant path of G contributes to $f(G)$ at least $\min\{\frac{(1-3)^2}{(1)(3)(1+3)}, \frac{(1-2)^2}{(1)(2)(1+2)} + \frac{(2-3)^2}{(2)(3)(2+3)}\} = \frac{1}{5}$ with equality if and only if the length of the path is at least two and the degree of its root is three.

So, $f(G) \geq \frac{3}{5}$ with equality if and only if G has exactly three pendant paths and each of them has length at least two, i.e., G is the trees with a single vertex of maximum degree three, adjacent to three vertices of degree two.

(ii) If $f(G) > \frac{3}{5}$, then G has exactly three pendant paths and at least one of them has length one, or G has at least four pendant paths. And $f(G) \geq \frac{2}{5} + \frac{1}{3} = \frac{11}{15}$ or $f(G) \geq \frac{4}{5} > \frac{11}{15}$. So, $f(G) \geq \frac{11}{15} > \frac{3}{5}$ with left equality if and only if G has exactly three pendant paths and exactly two of them have length at least two, i.e., G is the trees with a single vertex of maximum degree three, adjacent to one vertex of degree one and two vertices of degree two.

(iii) If $f(G) > \frac{11}{15}$, then G has exactly three pendant paths and at least two of them has length one, or G has at least four pendant paths. And $f(G) \geq \frac{1}{5} + \frac{2}{3} = \frac{13}{15} > \frac{4}{5}$ or $f(G) \geq \frac{4}{5}$. So, $f(G) \geq \frac{4}{5} > \frac{11}{15}$ with left equality if and only if G has exactly four pendant paths of length at least two and the maximum degree is three, the contribution to $f(G)$ of other edges is zero, i.e., G is the trees with exactly two adjacent vertices of maximum degree three, each adjacent to two vertices of degree two.

(iv) If $f(G) > \frac{4}{5}$, we distinguish them into three cases.

Case 1. G has exactly three pendant paths, then, by (i) and (ii), at least two of them has length one, and $f(G) \geq \frac{1}{5} + \frac{2}{3} = \frac{13}{15}$.

Case 2. G has exactly four pendant paths, then, by (iii), at least one of them has length one, or each of them has length two and G has two non-adjacent vertices of maximum degree three, or G has the maximum degree is at least four. $f(G) \geq \frac{3}{5} + \frac{1}{3} = \frac{14}{15} > \frac{13}{15}$, or $f(G) \geq \frac{4}{5} + 2[\frac{(2-3)^2}{(2)(3)(2+3)}] = \frac{13}{15}$, or $f(G) \geq 4\left[\frac{(1-2)^2}{(1)(2)(1+2)} + \frac{(2-4)^2}{(2)(4)(2+4)}\right] = 1 > \frac{13}{15}$.

Case 3. G has at least five pendant paths, then $f(G) \geq \frac{5}{5} > \frac{13}{15}$.

So, $f(G) \geq \frac{13}{15} > \frac{4}{5}$ with left equality if and only if G has exactly three pendant paths and at least two of them has length one, or G has two non-adjacent vertices of maximum degree three and exactly four pendant paths, each of them has length two, i.e., G is the trees with exactly two vertices of maximum degree three, each adjacent to three vertices of degree two, or the trees with a single vertex of maximum degree three, adjacent to two vertices of degree one and one vertex of degree two.

From (7), we know that the regular graph has the maximum harmonic index among all $n-$vertex graphs. So, among the $n-$vertex unicyclic graphs with $n \geq 3$, the cycle C_n is the unique graph with the maximum harmonic index, which is equal to $\frac{n}{2}$. Here, we will determine the $n-$vertex unicyclic graphs with the second for $n \geq 5$, the third for $n \geq 5$, the fourth for $n \geq 7$, and the fifth for $n \geq 8$ maximum harmonic indices.

Proposition 2. *Among the $n-$vertex unicyclic graphs,*
(i) For $n \geq 5$, the graph obtained from a cycle by attaching a pendant path of length at least two is the unique graphs with the second maximum harmonic index, which is equal to $\frac{n}{2} - \frac{2}{15}$.
(ii) For $n \geq 5$, the graph obtained from a cycle by attaching a pendant edge is the unique graph with the third maximum harmonic index, which is equal to $\frac{n}{2} - \frac{3}{15}$.
(iii) For $n \geq 7$, the graphs obtained from a cycle by attaching a pendant path of length at least two to two adjacent vertices of the cycle, respectively, or obtained by connecting an edge uv between a cycle and a path (where u is a vertex of the cycle, v is a vertex of the path and v is not adjacent to any pendant vertex) are the unique graphs with the fourth maximum harmonic index, which is equal to $\frac{n}{2} - \frac{7}{30}$.
(iv) For $n \geq 8$, the graphs obtained from a cycle by attaching a pendant path of length at least two to two non-adjacent vertices of the cycle, respectively, are the unique graphs with the fifth maximum harmonic index, which is equal to $\frac{n}{2} - \frac{4}{15}$.
(v) For $n \geq 9$, the graphs obtained by attaching a pendant path of length at least two to each vertex of C_3 are the unique graphs with the sixth maximum harmonic index, which is equal to $\frac{n}{2} - \frac{3}{10}$.

Proof. Let G be an $n-$vertex unicyclic graph different from C_n, where $n \geq 3$.

Note that the contribution to $f(G)$ of any edge in G is non-negative, and a pendant path of G contributes to $f(G)$ at least $\frac{1}{5}$.

If there is exactly one pendant path in G, then $f(G) \geq 2[\frac{(2-3)^2}{(2)(3)(2+3)}] + [\frac{(1-3)^2}{(1)(2)(1+2)}] = \frac{2}{5} = \frac{6}{15}$ with equality if and only if G is obtained from a cycle by attaching a pendant edge, or $f(G) \geq 3\left[\frac{(2-3)^2}{(2)(3)(2+3)}\right] + \left[\frac{(1-2)^2}{(1)(2)(1+2)}\right] = \frac{4}{15}$ with equality if and only if G is obtained from a cycle by attaching a pendant path of length at least two.

If there are at least three pendant paths in G, then $f(G) \geq \frac{3}{5} = \frac{9}{15}$ with equality if and only if the contribution to $f(G)$ of each pendant path is $\frac{1}{5}$ and the contribution to $f(G)$ of other edges is zero, i.e., G is obtained from C_3 by attaching a pendant path of length at least two to each vertex of C_3.

If there are exactly two pendant paths in G, then their roots are both on the cycle, or neither of them is on the cycle. There are the following cases:

(a) The two pendant paths have a common root on the cycle, then $f(G) \geq 2\left(\frac{(1-2)^2}{(1)(2)(1+2)}\right) + 4\left(\frac{(2-4)^2}{(2)(4)(2+4)}\right) = \frac{2}{3} = \frac{10}{15}$, since $\left(\frac{(1-4)^2}{(1)(4)(1+4)}\right) = \frac{9}{20} > \left(\frac{(1-2)^2}{(1)(2)(1+2)}\right) + \left(\frac{(2-4)^2}{(2)(4)(2+4)}\right) = \frac{1}{4}$.

(b) The roots of the two pendant paths are two adjacent vertices on the cycle, then $f(G) \geq 4[\frac{(2-3)^2}{(2)(3)(2+3)}] + 2[\frac{(1-2)^2}{(1)(2)(1+2)}] = \frac{7}{15}$ with equality if and only if G is obtained from a cycle by attaching a pendant path of length at least two to two adjacent vertices of the cycle, respectively.

(c) The roots of the two pendant paths are two non-adjacent vertices on the cycle, then $f(G) \geq 6[\frac{(2-3)^2}{(2)(3)(2+3)}] + 2[\frac{(1-2)^2}{(1)(2)(1+2)}] = \frac{8}{15}$ with equality if and only if G is obtained from a cycle by attaching a pendant path of length at least two to two non-adjacent vertices of the cycle, respectively.

(d) Neither of their roots is on the cycle, then they have a common root not on the cycle. We have $f(G) \geq 4[\frac{(2-3)^2}{(2)(3)(2+3)}] + 2[\frac{(1-2)^2}{(1)(2)(1+2)}] = \frac{7}{15}$ with equality if and only if G is obtained by connecting an edge uv between a cycle and a path, where u is a vertex of the cycle, v is a vertex of the path and v is not adjacent to any pendant vertex.

From the above arguments and $\frac{4}{15} < \frac{6}{15} < \frac{7}{15} < \frac{8}{15} < \frac{9}{15} < \frac{10}{15}$, we can obtain the results in Proposition 2.

In the following, we consider the harmonic indices of bicyclic graphs.

Let $B_1(r, s, t)$ be the bicyclic graph obtained from two vertex-disjoint cycles $C_r = u_1u_2 \cdots u_ru_1$ and $C_s = v_1v_2 \cdots v_sv_1$ by joining vertices u_1 and v_1 with a path $u_1w_1 \cdots w_{t-1}v_1$ of length t, where $r, s \geq 3$, $t \geq 0$.

Let $A_1(r, s, k)$ be the bicyclic graph obtained from $B_1(r, s, 1)$ by attaching a pendant path of length k to the vertex v_2.

Let $A_2(r, s, k)$ be the bicyclic graph obtained from $B_1(r, s, 2)$ by attaching a pendant path of length k to the vertex w_1.

Let $B_2(a, b, c)$ be the bicyclic graph obtained from three paths $u_0u_1 \cdots u_a$, $v_0v_1 \cdots v_b$ and $w_0w_1 \cdots w_c$ by identifying $u_0 = v_0 = w_0$ and $u_a = v_b = w_c$, respectively, where $1 \le a = \min\{a, b, c\}$.

Let $A_3(b, c, k)$ be the bicyclic graph obtained from $B_2(2, b, c)$ by attaching a pendant path of length k to the vertex u_1.

Let $A_4(b, c, k)$ be the bicyclic graph obtained from $B_2(1, b, c)$ by attaching a pendant path of length k to the vertex v_1.

Let $A_5(c, k)$ be the bicyclic graph obtained from $B_2(1, 2, c)$ by attaching a pendant path of length k to the vertex v_1.

Proposition 3. *we assume that $k \ge 2$ in the following. Among the $n-$vertex bicyclic graphs,*
(i) For $n \ge 6$, the graphs $B_1(r, s, 1)$ (where $r+s = n$) and $B_2(1, b, c)$ (where $b + c = n$ and $b, c \ge 2$) are the unique $n-$vertex bicyclic graphs with the maximum harmonic index, which is equal to $\frac{n}{2} - \frac{2}{30}$.
(ii) For $n \ge 7$, the graphs $B_1(r, s, t)$ (where $r + s + t - 1 = n$, $t \ge 2$) and $B_2(a, b, c)$ (where $a + b + c = n + 1$, $a \ge 2$) are the unique graphs with the second maximum harmonic index, which is equal to $\frac{n}{2} - \frac{1}{10}$.
(iii) For $n \ge 7$, the graphs $A_5(c, k)$ (where $c + 2 + k = n$ and $c \ge 2$) are the unique graphs with the third maximum harmonic index, which is equal to $\frac{n}{2} - \frac{2}{15}$.
(iv) For $n \ge 9$, the graphs $B_1(r, s, 0)$ (where $r + s - 1 = n$), $A_1(r, s, k)$ (where $r + s + k = n$), $A_2(r, s, k)$ (where $r + s + k + 1 = n$), $A_3(b, c, k)$ (where $b + c + 1 + k = n$) and $A_4(b', c', k)$ (where $b' \ge 3$, $b' + c' + k = n$) are the two graphs with the fourth maximum harmonic index, which is equal to $\frac{n}{2} - \frac{1}{6}$.

Proof. First, for the bicyclic graphs with no pendant vertices, we have $f(B_1(r, s, 1)) = f(B_2(1, b, c)) = \frac{2}{15}$, $f(B_1(r, s, t)) = f(B_2(a, b, c)) = \frac{1}{5}$, where $t \ge 2$, $a \ge 2$, and $f(B_1(r, s, 0)) = \frac{1}{3}$.

Second, we consider the bicyclic graphs with one pendant vertex.

If G is obtained from $B_1(r, s, 0)$ by attaching a pendant path, then $f(G) > \frac{1}{3}$.

If G is obtained from $B_1(r, s, 1)$ by attaching a pendant path, then $f(G) \ge \frac{1}{3}$ with equality if and only if $G \cong A_1(r, s, k)$, where $k \ge 2$.

If G is obtained from $B_1(r, s, t)$ (where $t \ge 2$) by attaching a pendant path, then $f(G) \ge \frac{1}{3}$ with equality if and only if $G \cong A_2(r, s, k)$, where $k \ge 2$.

If G is obtained from $B_2(1, b, c)$ by attaching a pendant path, then $f(G) = \frac{4}{15}$ for $G \cong A_5(c, k)$, and $f(G) \ge \frac{1}{3}$ for $G \ncong A_5(c, k)$, with equality if and only if $G \cong A_4(b, c, k)$, where $k \ge 2$.

If G is obtained from $B_2(a, b, c)$ (where $a \ge 2$) by attaching a pendant path, then $f(G) \ge \frac{1}{3}$ with equality if and only if $G \cong A_3(b, c, k)$, where $k \ge 2$.

Third, for any bicyclic graph G with at least two pendant vertices, we have $f(G) \geq \frac{2}{5}$ since every pendant path of G contributes to $f(G)$ at least $\frac{1}{5}$.

From the above arguments and $\frac{2}{15} < \frac{1}{5} < \frac{4}{15} < \frac{1}{3} < \frac{2}{5}$, we can obtain the results in Proposition 3.

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