On the harmonic index of the unicyclic and bicyclic graphs

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Abstract: The harmonic index is one of the most important indices in chemical and mathematical fields. It's a variant of the Randić index which is the most successful molecular descriptor in structure-property and structure-activity relationships studies. The harmonic index gives somewhat better correlations with physical and chemical properties comparing with the well known Randić index. 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. In this paper, we present the unicyclic and bicyclic graphs with minimum and maximum harmonic index, and also characterize the corresponding extremal graphs. The unicyclic and bicyclic graphs with minimum harmonic index are S_n^+, S_n^1 respectively, and the unicyclic and bicyclic graphs with maximum are C_n, B_n or B_n' respectively. As a simple result, we present a short proof of one theorem in Applied Mathematics Letters 25 (2012) 561-566, that the trees with maximum and minimum harmonic index are the path P_n and the star S_n, respectively. Moreover, we give a further discussion about the property of the graphs with the maximum harmonic index, and show that the regular or almost regular graphs have the maximum harmonic index in connected graphs with n vertices and m edges.

Key–Words: The harmonic index; minimum; maximum; unicyclic graphs; bicyclic graphs

1 Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. A single number which characterizes the graph of a molecular is called a graph-theoretical invariant or topological index. The structure property relationship quantity the connection between the structure and properties of molecules. In 1975, Randić proposed a new structural descriptor [23], which is defined as the sum of the weights $(d(u)d(v))^{-\frac{1}{2}}$ of all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G. It is defined as follows:

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

At first, he called it the branching index, but later it was renamed to the connectivity index [16, 17] or Randić index [21, 25]. Randić himself demonstrated that the index had been closed correlated with a variety of physico-chemical proper ties of alkanes, such as boiling point, (experimental), kova'ts index, enthalpy of formation, parameters in the Antoine equation (for vapour pressure), surface area, and solubility in water, see [23]. The Randić index is one of the most successful molecular descriptors in structure-property and structure-activity relationships studies, suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. Like other successful chemical indices, this index has received considerable attentions from chemists and mathematicians [10, 13, 14, 20] and been successfully related to a variety of physical, chemical and pharmacological properties of organic molecules.

Later, the Randić connectivity index had been extended as the general Randić connectivity index by replacing $-\frac{1}{2}$ with any real number α, it's defined as

$$R_\alpha(G) = \sum_{uv\in E(G)} (d(u)d(v))^{\alpha}.$$

where $\alpha(\alpha \neq 0)$ is an arbitrary real number. Recently $R_\alpha(G)$ has received considerable attentions in mathematical literature cf. e.g.[2, 3]. For $\alpha = 1$, one obtains second Zagreb index, M_2 [11]; for $\alpha = -1$, one obtains modified Zagreb index [22], etc.

With motivation from the Randić index, a closely related variant of the Randić connectivity index called the sum-connectivity index was recently proposed by Zhou and Trinajstić [28] in 2009. The sum-connectivity index $\chi(G)$ was defined as follows:

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

and the general sum-connectivity index $\chi_\alpha(G)$ was defined as follows:

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

where $\alpha(\alpha \neq 0)$ is an arbitrary real number. $\chi(G)$ is a graph-based molecular structure descriptor. The sum-connectivity index has been found to correlate well with π-electronic energy of benzenoid hydrocarbons. In [18], they use both the Randić index and the sum-connectivity index to approximate rather accurately the π-electron energy (E_π) of benzenoid hydrocarbons. The correlation coefficients between $\chi(G)$ and E_π, and $R(G)$ and E_π are 0.9999 and 0.9992, respectively. The value of the correlation coefficient is 0.99088 for 136 trees representing the lower alkanes taken from Ivanciuc *et. al.* [15]. It shows that the sum-connectivity index and original Randić connectivity index are highly intercorrelated molecular descriptors. The sum-connectivity index is frequently applied in quantitative structure-property and structure-activity studies [4, 12, 17, 19, 24]. Some mathematical properties of the sum-connectivity and general sum-connectivity are given in [5, 6, 7, 27, 29].

Then D. Vukičević and B. Furtula introduce another novel topological index based on the end-vertex degrees of edges which is named as geometrical-arithmetic connectivity index (GA) [26], which is defined as

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

From the definition, we can see that this index consists from geometrical mean of end-vertex degrees of an edge uv as numerator and arithmetic mean of end-vertex degrees of the edge uv as denominator.

Predictive power of this index has been tested on some physico-chemical properties of octanes. From the website *www.moleculardescriptors.eu*, we can see the results and the models of boiling point, entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation, acentric factor. Obtained results show that it gives somewhat better results than the well-known Randić connectivity index, we can see the details in [26]. The prediction power of GA index is at least for 2.5% better than power of Randić index. The greatest improvement in prediction with GA index comparing to Randić index is obtained in the case of standard enthalpy of vaporization, which is more than 9%.

Another variant of the Randić index named the harmonic index which first appeared in [9]. For a graph G, the harmonic index $H(G)$ is defined as

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

When comparing $H(G)$ to $R(G)$, it's easy to see that $H(G) \leq R(G)$ with equality if and only if G is a regular graph. The regular graphs have turned out to be the extremal graphs with the maximum value of the harmonic index. For any graph G, we can see that when $\alpha = 1$, $H(G) = 2\chi_1(G)$. Favaron *et. al.* [8] considered the relationship between the harmonic index and the eigenvalues of graphs. Zhong [30] considers the minimum and maximum values of the harmonic index for simple connected graphs and trees, and characterizes the corresponding extremal graphs. It turns out that the trees with maximum and minimum harmonic index are the path P_n and the star S_n, respectively. And the star S_n also reaches the minimum harmonic index in simple connected graphs.

In this paper, we firstly give two crucial lemmas. As a result, we present a short proof of the theorem in [30] which deduced the path P_n has the maximum harmonic index. Then we consider the unicyclic and bicyclic graphs, and show the sharp lower and upper bound on the harmonic index of unicyclic and bicyclic graphs. The corresponding graphs which reach the bounds are given as follows. The unicyclic and bicyclic graphs with minimum values of the harmonic index are S_n^+, S_n^1, respectively, and the maximum C_n, B_n or B'_n, respectively. Finally we give a further discussion about the property of the graphs with the maximum harmonic index by analyzing the variables of the formula of harmonic index. We show that the regular or almost regular graphs have the maximum harmonic index among all connected graphs with n vertices and m edges.

2 Preliminaries

Before proceeding, we introduce some notations and terminology. Throughout this paper, we only consider simple and loopless graphs. For a graph G, let $d_G(u)$ be the degree of a vertex u in G. We can omit the subscript if there is no ambiguity. Denote by $\Delta(G)$ the maximum degree of G, and $\delta(G)$ the minimum degree of G. Let $N(u)$ be the neighbors (i.e. the vertices adjacent to u) of u. If $d(u) = 1$, then u is said to be a *pendent vertex* in G, and the edge incident with u is referred to as *pendent edge*. The neighbor of a pendent vertex is called a *support vertex*. The *distance* between u and v in graph G, denoted by $d(u, v)$, is the length of shortest (u, v)-path in G. The *diameter* of G, denoted by $D(G)$, is the maximum distance between any two vertices. For an edge $e = uv$, the *weight* of e in G is $w_G(e) = \frac{2}{d(u)+d(v)}$. Denote by, as usual, P_n, S_n and C_n the path, the star and the cycle on n vertices, respectively. A *unicyclic graph* is a connected graph with n vertices and n edges. A *bicyclic graph* of order n is a connected graph with n vertices and $n + 1$ edges. If $\delta(G) = \Delta(G)$, then G is called a regular graph, if $\delta(G) = \Delta(G) - 1$, then G is a almost regular graph. Other notations and terminology undefined here referred to [1].

Throughout this paper, the following two lemmas are crucial.

Lemma 1 *Let G be a graph of order $n \geq 4$. If there is an edge uv with $d(u) \geq 2$ and $d(v) \geq 2$, and $N(u) \cap N(v) = \emptyset$. By contracting uv to u' and adding a pendent edge $u'v'$ on u', we get a new graph G'. Then we have $H(G') < H(G)$.*

Proof: Suppose $N(u) \setminus \{v\} = \{x_1, x_2, \cdots, x_{d(u)-1}\}$, $N(v) \setminus \{u\} = \{y_1, y_2, \cdots, y_{d(v)-1}\}$. Since $d(u) \geq 2$, $d(v) \geq 2$, we have $d(u) - 1 > 0$, and $d(v) - 1 > 0$. Then

$$\begin{aligned}
& H(G') - H(G) \\
= \; & \frac{2}{d(u) + d(v) - 1 + 1} - \frac{2}{d(u) + d(v)} \\
& + \sum_{i=1}^{d(u)-1} \frac{2}{d(u) + d(v) - 1 + d(x_i)} \\
& + \sum_{i=1}^{d(v)-1} \frac{2}{d(u) + d(v) - 1 + d(y_j)} \\
& - \sum_{i=1}^{d(u)-1} \frac{2}{d(u) + d(x_i)} - \sum_{j=1}^{d(v)-1} \frac{2}{d(v) + d(y_i)} \\
= \; & \sum_{i=1}^{d(u)-1} \left(\frac{2}{d(u) + d(x_i) + d(v) - 1} - \frac{2}{d(u) + d(x_i)}\right) \\
& + \sum_{i=1}^{d(v)-1} \left(\frac{2}{d(v) + d(y_j) + d(u) - 1} - \frac{2}{d(v) + d(y_i)}\right) \\
< \; & 0.
\end{aligned}$$

So we have $H(G') < H(G)$. □

Lemma 2 *Let G be a n-vertex graph ($n \geq 5$) with at least two pendent vertices, say s and t, and $\Delta(G) > 2$. Let u be a vertex with maximum degree, and v be a neighbor of u with $d(v) = \max\{d(v_i), v_i \in N(u)\}$. Let $G' := G - uv + st$. If the new graph G' is connected, then we have $H(G') > H(G)$.*

Proof: Suppose $N(u) \setminus \{v\} = \{x_1, x_2, \cdots, x_{d(u)-1}\}$, $N(v) \setminus \{u\} = \{y_1, y_2, \cdots, y_{d(v)-1}\}$. Let a, b be the support vertex of s, t, respectively. Let's consider the weights of as and bt. If $a = u$, then $w_G(as) = w_{G'}(as)$. The case for $b = v$ is similar. So without lose of generality, we can assume that $a \neq u$, and $b \neq v$.

$$\begin{aligned}
& H(G') - H(G) \\
= \; & \sum_{e \in E(G')} w_{G'}(e) - \sum_{e \in E(G)} w_G(e) \\
= \; & \frac{2}{2+2} - \frac{2}{d(u) + d(v)} + \frac{2}{d(a) + 2} + \frac{2}{d(b) + 2} \\
& - \frac{2}{d(a) + 1} - \frac{2}{d(b) + 1} \\
& + \sum_{i=1}^{d(u)-1} (w_{G'}(ux_i) - w_G(ux_i)) \\
& + \sum_{j=1}^{d(v)-1} (w_{G'}(vy_j) - w_G(vy_j))
\end{aligned}$$

By the choices of u, v, we have $d(x_i) \leq d(v), i \in \{1, 2, \cdots, d(u) - 1\}$, and $d(y_j) \leq d(u), j \in \{1, 2, \cdots, d(v) - 1\}$. So

$$\begin{aligned}
& w_{G'}(ux_i) - w_G(ux_i) \\
= \; & \frac{2}{d(u) - 1 + d(x_i)} - \frac{2}{d(u) + d(x_i)} \\
= \; & \frac{2}{(d(u) + d(x_i))(d(u) - 1 + d(x_i))} \\
\geq \; & \frac{2}{(d(u) + d(v))(d(u) - 1 + d(v))}
\end{aligned}$$

$$\begin{aligned}
& w_{G'}(vy_j) - w_G(vy_j) \\
= \; & \frac{2}{d(v) - 1 + d(y_j)} - \frac{2}{d(v) + d(y_j)} \\
= \; & \frac{2}{(d(v) + d(y_j))(d(v) - 1 + d(y_j))} \\
\geq \; & \frac{2}{(d(u) + d(v))(d(u) - 1 + d(v))}
\end{aligned}$$

Then

$$\begin{aligned}
& H(G') - H(G) \\
\geq \; & \frac{1}{2} - \frac{2}{(d(u) + d(v))(d(u) - 1 + d(v))} \\
- \; & \frac{2}{(d(a) + 1)(d(a) + 2)} - \frac{2}{(d(b) + 1)(d(b) + 2)}
\end{aligned}$$

Since $d(a), d(b) \geq 2$, then we have

$$\frac{2}{(d(a)+1)(d(a)+2)} \leq \frac{1}{6},$$

and

$$\frac{2}{(d(b)+1)(d(b)+2)} \leq \frac{1}{6}.$$

Moreover, $d(u) \geq 3, d(v) \geq 1$. But the equalities can not hold simultaneously. Therefore,

$$\frac{2}{(d(u)+d(v))(d(u)-1+d(v))} < \frac{1}{6}.$$

So we have $H(G') - H(G) > 0$. □

Using this lemma, we can easily prove that the path P_n has the maximum harmonic index, which showed by Zhong in [30].

Remark 3 *Among the trees of order n, the path P_n has the maximum harmonic index.*

Proof: It is trivial when $n = 3, 4$. Now we assume $n \geq 5$ and induce the proof by contradiction. Let T be the tree with maximum harmonic index. If $T \neq P_n$, then $\Delta(T) > 2$. Let uv be the edge satisfying Lemma 2. As T is a tree, it is easy to find two leaves s and t in each component of $T - uv$. So $T' = T - uv + st$ is connected. From Lemma 2, we have $H(T') > H(T)$. This contradicts to the choice of T. □

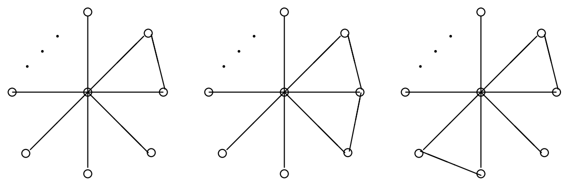
3 The minimum values of the harmonic index for unicyclic and bicyclic graphs

The unicyclic graph S_n^+ is obtained from the star S_n by adding an edge joining two pendent vertices. The bicyclic graph S_n^1 is obtained from the S_n by adding a path of length 2 joining three pendent vertices. And the bicyclic graph S_n^2 is obtained from the S_n by adding two edges joining two different pairs of pendent vertices, see Figure 1.

We will show that S_n^+ and S_n^1 have the minimum values of the harmonic index for unicyclic and bicyclic graphs, respectively.

Theorem 4 *Let G be a unicyclic graph of order $n \geq 3$. Then $H(G) \geq H(S_n^+) = \frac{5n^2+n-12}{2n(n+1)}$ with equality if and only if $G \cong S_n^+$.*

Proof: Clearly, $H(S_n^+) = \frac{5n^2+n-12}{2n(n+1)}$. It is easy to prove that the theorem holds for $n = 3, 4$. Now we assume $n \geq 5$. Suppose for a contradiction that there is a unicyclic graph G_0 ($G_0 \neq S_n^+$) has the minimum value of the harmonic index.



${S_n}^+$ ${S_n}^1$ ${S_n}^2$

Figure 1: The unicyclic graph S_n^+, and the bicyclic graphs S_n^1, S_n^2

Since $n \geq 5$ and $G_0 \neq S_n^+$, then we have $D(G_0) > 2$. There must be a path P of length at least 3 in G_0. Let uv be an edge in P with $d(u) \geq 2$, $d(v) \geq 2$. If $N(u) \cap N(v) = \emptyset$, by Lemma 1, we can get a new graph G_0', such that $H(G_0') < H(G_0)$, a contradiction.

If $N(u) \cap N(v) \neq \emptyset$, there is only one vertex $w \in N(u) \cap N(v)$, for unicyclic graph G_0. We claim that the edges incident with $\{u, v, w\}$, other than uv, vw and uw, are all pendent edges. For otherwise, as the cycle uvw is the unique cycle in G_0, there is an edge satisfying the condition of Lemma 1. We can get a new graph G_0', such that $H(G_0') < H(G_0)$, a contradiction. So, without lose of generality, we can assume that $d(u) \geq d(v) \geq d(w) \geq 2$, and $d(u) \geq 3$. By deleting the pendent edges incident to v and adding them on u, we get a new graph G_0'. So

$$\begin{aligned}
& H(G_0') - H(G_0) \\
= \ & \frac{2(d(u)+d(v)-4)}{d(u)+d(v)-2+1} + \frac{2}{d(w)+2} \\
& -\frac{2(d(u)-2)}{d(u)+1} + \frac{2}{d(u)+d(v)-2+d(w)} \\
& -\frac{2}{d(u)+d(w)} - \frac{2}{d(v)+d(w)} - \frac{2(d(v)-2)}{d(v)+1} \\
\leq \ & \frac{6(d(v)-2)}{(d(u)+1)(d(u)+d(v)-1)} \\
& + \frac{2(d(v)-2)}{(d(v)+d(w))(d(w)+2)} - \frac{2(d(v)-2)}{d(v)+1} \\
\leq \ & \frac{2(d(v)-2)}{d(v)+2} - \frac{2(d(v)-2)}{d(v)+1} < 0
\end{aligned}$$

This contradiction completes the proof. □

Theorem 5 *Let G be a bicyclic graph of order $n \geq 4$. Then $H(G) \geq H(S_n^1) = \frac{14}{5} - \frac{2n^2+14n+16}{n(n+1)(n+2)}$ with equality if and only if $G \cong S_n^1$.*

Proof: It is trivial for $n = 4, 5$. Now we assume $n \geq 6$. Clearly, $H(S_n^1) = \frac{14}{5} - \frac{2n^2+14n+16}{n(n+1)(n+2)}$. Suppose for a contradiction that there is a bicyclic graph G_0 ($G_0 \neq S_n^1$) has the minimum value of the harmonic index. Note that, there are only two non-isomorphic bicyclic graphs with diameter 2. One is S_n^1 and the other is S_n^2. Since $H(S_n^2) = \frac{3n^2+n-10}{n(n+1)} > H(S_n^1)$. Then we can assume that $D(G_0) > 2$. Furthermore, if there is an edge uv in G_0 with $d(u) \geq 2$, $d(v) \geq 2$, and $N(u) \cap N(v) = \emptyset$. Then by Lemma 1, we can get a new graph G_0', such that $H(G_0') < H(G_0)$. It contradicts to the choice of G_0. So we conclude that the edge in G_0 is either pendent edge or in a triangle C_3. In addition, there are only two triangles in G_0. We distinguish two cases.

Case1. The two triangles share a common vertex, say u.

In this case, there are only five vertices are non-pendent vertices. Denote by uvx_1 and ux_2x_3 the two triangles in G_0. Without lose of generality, we can assume $d(v) \geq d(x_1)$ and $d(x_2) \geq d(x_3)$.

If $d(x_1) > 2$ (the case for $d(x_3) > 2$ is similar). By deleting the pendent edges incident with x_1 and adding them on v, we get a new graph G_0'. Then

$$
\begin{aligned}
& H(G_0') - H(G_0) \\
= \; & \frac{2}{d(u)+d(v)+d(x_1)-2} + \frac{2}{d(u)+2} \\
& + \frac{2(d(v)+d(x_1)-4)}{d(v)+d(x_1)-1} - \frac{2}{d(u)+d(v)} \\
& - \frac{2}{d(u)+d(x_1)} - \frac{2(d(v)-2)}{d(v)+1} - \frac{2(d(x_1)-2)}{d(x_1)+1} \\
= \; & \frac{2(d(v)-2)}{(d(u)+2)(d(u)+d(v))} - \frac{2(d(v)-2)}{d(v)+1} \\
& - \frac{2(d(v)-2)}{(d(u)+d(v)+d(x_1)-2)(d(u)+d(x_1))} \\
& + \frac{6(d(v)-2)}{(d(v)+d(x_1)-1)(d(x_1)+1)}
\end{aligned}
$$

Since $d(v) \geq d(x_1) \geq 3$ and $d(u) \geq 4$,

$$
\begin{aligned}
& H(G_0') - H(G_0) \\
\leq \; & \frac{2(d(v)-2)}{(d(u)+2)(d(u)+d(v))} \\
& - \frac{2(d(v)-2)}{(d(u)+2d(v)-2)(d(u)+d(v))} \\
& + \frac{3(d(v)-2)}{2(d(v)+2)} - \frac{2(d(v)-2)}{d(v)+1} \\
= \; & \frac{4(d(v)-2)^2}{(d(u)+2)(d(u)+d(v))(d(u)+2d(v)-2)} \\
& - \frac{(d(v)+5)(d(v)-2)}{2(d(v)+1)(d(v)+2)} \\
\leq \; & \frac{(d(v)-2)^2}{3(d(v)+1)(d(v)+4)} - \frac{(d(v)+5)(d(v)-2)}{2(d(v)+1)(d(v)+2)} \\
= \; & \frac{(d(v)-2)(-d(v)^2-27d(v)-68)}{6(d(v)+1)(d(v)+2)(d(v)+4)} < 0
\end{aligned}
$$

So $H(G_0') < H(G_0)$, a contradiction.

Thus we have $d(x_1) = d(x_3) = 2$. Since $D(G_0) > 2$, then without lose of generality we can assume $d(v) > 2$. By deleting the pendent edges incident with v and adding them on u, we get a new graph G_0'. Then

$$
\begin{aligned}
& H(G_0') - H(G_0) \\
= \; & \frac{2}{d(u)+d(v)+d(x_2)-2} \\
& - \frac{2}{d(u)+d(x_2)} + \frac{4}{d(u)+d(v)} - \frac{4}{d(u)+2} \\
& + \frac{2(d(u)+d(v)-6)}{d(u)+d(v)-1} - \frac{2(d(u)-4)}{d(u)+1} + \frac{1}{2} \\
& - \frac{2}{d(v)+2} - \frac{2(d(v)-2)}{d(v)+1} \\
< \; & \frac{10(d(v)-2)}{(d(u)+1)(d(u)+d(v)-1)} - \frac{d(v)-2}{2d(v)+4} \\
& - \frac{2(d(v)-2)}{d(v)+1} \\
< \; & \frac{2(d(v)-2)}{d(v)+3} - \frac{2(d(v)-2)}{d(v)+1} < 0
\end{aligned}
$$

Since $d(u) \geq 4$, we get $H(G_0') < H(G_0)$. It is a contradiction.

Case 2. The two triangles share a common edge, say uv.

In this case, there are only four vertices are non-pendent vertices. Let w, x be the common neighbors of u and v. We can assume that $d(u) \geq d(v) \geq 3, d(x) \geq d(w) \geq 2$.

Subcase 1. $d(x) = 2$.

Then $d(w) = 2$. In this case $d(u) \geq d(v) \geq 4$ for $G_0 \neq S_n^1$. Then by deleting the pendent edges incident to v and adding them on u, we get a new graph G_0'. Then

$$H(G_0') - H(G_0)$$

$$\begin{aligned}
&= \frac{4}{d(u)+d(v)-1}+\frac{4}{5}+\frac{2(d(u)+d(v)-6)}{d(u)+d(v)-2} \\
&\quad -\frac{2(d(u)-3)}{d(u)+1}-\frac{2(d(v)-3)}{d(v)+1}-\frac{4}{d(u)+2} \\
&\quad -\frac{4}{d(v)+2} \\
&< \frac{8(d(v)-3)}{(d(u)+d(v)-2)(d(u)+1)} \\
&\quad +\frac{4(d(v)-3)}{5(d(v)+2)}-\frac{2(d(v)-3)}{d(v)+1} \\
&< \frac{4(d(v)-3)}{d(v)^2-1}+\frac{4(d(v)-3)}{5(d(v)+2)}-\frac{2(d(v)-3)}{d(v)+1} \\
&= (d(v)-3)\left(\frac{-6d(v)^2+10d(v)+56}{5(d(v)^2-1)(d(v)+2)}\right) \\
&\leq 0
\end{aligned}$$

We get $H(G_0') < H(G_0)$, a contradiction.

Subcase 2. $d(u) = 3$

Then $d(v) = 3$ too. If $d(w) = 2$, then $d(x) \geq 3$ for $n \geq 6$. Thus

$$H(G_0) = \frac{47}{15} - \frac{2n+10}{n^2-1} > H(S_n^1),$$

a contradiction.

So we may assume $d(x) \geq d(w) \geq 3$. Then by deleting the pendent edges incident to w and adding them on x, we get a new graph G_0'. Then

$$\begin{aligned}
&H(G_0') - H(G_0) \\
&= \frac{4}{d(w)+d(x)+1}-\frac{4}{d(x)+3} \\
&\quad +\frac{2(d(w)+d(x)-4)}{d(w)+d(x)-1}-\frac{2(d(w)-2)}{d(w)+1} \\
&\quad -\frac{2(d(x)-2)}{d(x)+1}+\frac{4}{5}-\frac{4}{d(w)+3} \\
&< \frac{6(d(w)-2)}{(d(w)+d(x)-1)(d(x)+1)}+\frac{4(d(w)-2)}{5(d(w)+3)} \\
&\quad -\frac{2(d(w)-2)}{d(w)+1} \\
&\leq \frac{3\cdot 2(d(w)-2)}{(d(w)+1)(2d(w)-1)}+\frac{2\cdot 2(d(w)-2)}{5(d(w)+3)} \\
&\quad -\frac{2(d(w)-2)}{d(w)+1} \\
&= \frac{2(d(w)-2)(-6d(w)^2-8d(w)+58)}{5(d(w)+1)(d(w)+3)(2d(w)-1)} \\
&< 0
\end{aligned}$$

We get $H(G_0') < H(G_0)$, a contradiction.

Subcase 3. $d(x) \geq 3$ and $d(u) \geq 4$.

By deleting the pendent edges incident to x and adding them on u, we get a new graph G_0'. Then

$$\begin{aligned}
&H(G_0') - H(G_0) \\
&= \frac{2(d(u)+d(x)-5)}{d(u)+d(x)-1}+\frac{2}{d(v)+2} \\
&\quad +\frac{2}{d(u)+d(x)+d(w)-2}-\frac{2}{d(u)+d(v)} \\
&\quad +\frac{2}{d(u)+d(x)+d(v)-2}-\frac{2}{d(u)+d(w)} \\
&\quad -\frac{2}{d(x)+d(v)}-\frac{2(d(u)-3)}{d(u)+1}-\frac{2(d(x)-2)}{d(x)+1} \\
&< \frac{8d(x)-16}{(d(u)+d(x)-1)(d(u)+1)} \\
&\quad +\frac{2d(x)-4}{(d(v)+2)(d(x)+d(v))}-\frac{2d(x)-4}{d(x)+1}
\end{aligned}$$

Since $d(u) \geq 4$, $d(v) \geq 3$,

$$\begin{aligned}
&H(G_0') - H(G_0) \\
&\leq \frac{2d(x)-4}{5(d(x)+3)}+\frac{8d(x)-16}{5(d(x)+3)}-\frac{2d(x)-4}{d(x)+1} \\
&= \frac{2d(x)-4}{d(x)+3}-\frac{2d(x)-4}{d(x)+1} \\
&< 0
\end{aligned}$$

Then we have $H(G_0') < H(G_0)$, a contradiction generates. □

4 The maximum values of the harmonic index for unicyclic and bicyclic graphs

The bicyclic graph B_n is a bicyclic graph obtained by inserting an edge between two non-adjacent vertices of C_n, and B_n' is a bicyclic graph obtained by connecting two disjoint cycles by means of a new edge. Let Y_n be a bicyclic graph obtained by identifying any two vertices of two cycles. Let Y_n' be a bicyclic graph obtained by inserting a path of length at least two between two non-adjacent vertices of C_n. Let Y_n'' be a bicyclic graph obtained by connecting two disjoint cycles by means of a path of length at least two, see Figure 2.

Theorem 6 *Let G be a unicyclic graph of order $n \geq 3$, then $H(G) \leq H(C_n) = \frac{n}{2}$ with equality if and only if $G \cong C_n$.*

Proof: It is easy to prove that the theorem holds for $n = 3, 4$. Now we assume $n \geq 5$. Suppose for a

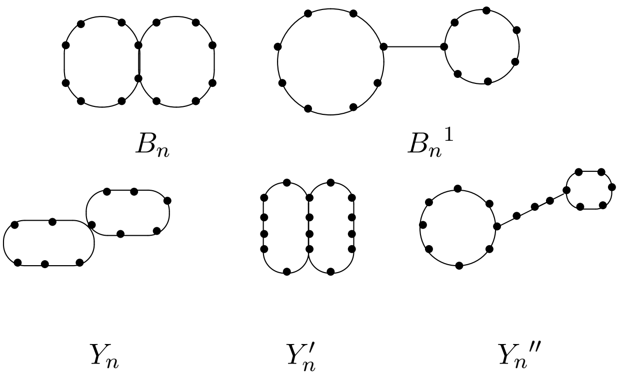


Figure 2: The bicyclic graphs B_n, B_n^1, Y_n, Y_n', and Y_n''

contradiction that there is a unicyclic graph $G \neq C_n$ has the maximum value of the harmonic index.

Case 1. If G has only one pendent vertex, say u.

Let v be the support vertex of u. If $d(v) = 3$, then $H(G) = \frac{n}{2} - \frac{1}{5} < H(C_n)$. If $d(v) = 2$, then $H(G) = \frac{n}{2} - \frac{2}{15} < H(C_n)$. Both contradict the choice of G.

Case 2. If G has at least two pendent vertices, say s and t.

Note that $\Delta(G) > 2$, for $G \neq C_n$. Let u be a vertex with maximum degree, and v be a neighbor of u with $d(v) = \max\{d(v_i), v_i \in N(u)\}$. Let $G' := G - uv + st$. If G' is connected, then by Lemma 2, we can get a new graph G' that $H(G') - H(G) > 0$. This contradicts to the choice of G.

So we conclude that $G - uv$ is disconnected and has two components G_1 and G_2, and $u \in G_1, v \in G_2$. Moreover, one of G_1 and G_2 has no pendent vertex for unicyclic graph $G \neq C_n$. Note that we take no account of u and v when consider the pendent vertex of G_1 and G_2. We distinguish two subcases.

Subcase 1. G_2 has no pendent vertex.

Then G_1 has at least a pendent vertex, say t. Let s be the support vertex of t. We do not exclude the possibility that $s = u$. Suppose $V(G_1) = n_1$, $E(G_1) = m_1, V(G_2) = n_2, E(G_2) = m_2$. Then we have $n_1 + n_2 = n, m_1 + m_2 = n - 1$.

Since G_2 has no pendent vertex. Then G_2 is not a tree. So $m_2 \geq n_2$. On the other hand, G_2 has at most one cycle, for G is a unicyclic graph. So $m_2 \leq n_2$. Then we have $m_2 = n_2$, furthermore, $m_1 = n_1 - 1$. Now we deduce that G_1 is a tree, whereas G_2 is a unicyclic graph with no pendent vertex. So $d_G(v) = 3$, if v is a vertex of cycle; while $d_G(v) = 2$, if v is a pendent vertex of G_2.

Let $G' := G - uv + tv$. Suppose $N(u) \setminus \{v\} = \{x_i, 1 \leq i \leq d(u) - 1\}$.

$$\begin{aligned}
& H(G') - H(G) \\
= & \sum_{i=1}^{d(u)-1} \left(\frac{2}{d(u) - 1 + d(x_i)} - \frac{2}{d(u) + d(x_i)}\right) \\
& + \frac{2}{d(v) + 2} - \frac{2}{d(u) + d(v)} \\
& + \frac{2}{d(s) + 2} - \frac{2}{d(s) + 1} \\
= & \sum_{i=1}^{d(u)-1} \frac{2}{(d(u) - 1 + d(x_i))(d(u) + d(x_i))} \\
& + \frac{2d(u) - 4}{(d(v) + 2)(d(u) + d(v))} \\
& - \frac{2}{(d(s) + 1)(d(s) + 2)}
\end{aligned}$$

Since $d(u) \geq d(x_i)$, and $d(s) \geq 2$

$$\begin{aligned}
& H(G') - H(G) \\
\geq & \frac{2d(u) - 4}{(d(v) + 2)(d(u) + d(v))} \\
& + \frac{2d(u) - 2}{(d(u) - 1 + d(v))((d(u) + d(v))} - \frac{1}{6}
\end{aligned}$$

Since $d(u) \geq 3$ and $d(v) = 2$ or $d(v) = 3$. So $H(G') - H(G) > 0$.

Subcase 2. G_1 has no pendent vertex.

Then G_2 has at least a pendent vertex t. Let s be the support vertex of t. We do not exclude the possibility that $s = v$. Similar to the discussion in Case 1, we have $m_1 = n_1$, and $m_2 = n_2 - 1$. So G_2 is a tree. Since u is the maximum vertex and G_1 has no pendent vertex, we can claim that G_1 is a cycle. Let w be a neighbor of u. Then $d(u) = 3$, and $d(w) = 2$. So $2 \leq d(s), d(v) \leq 3$. Let $G' := G - uw + tw$. We have

$$\begin{aligned}
& H(G') - H(G) \\
= & \; 2\left(\frac{2}{2+2} - \frac{2}{3+2}\right) + \frac{2}{d(v) + 2} \\
= & -\frac{2}{3 + d(v)} + \frac{2}{d(s) + 2} - \frac{2}{d(s) + 1} \\
& = \frac{1}{5} + \frac{2}{(d(v) + 2)(d(v) + 3)} \\
= & -\frac{2}{(d(s) + 1)(d(s) + 2)} \\
& \geq \frac{1}{5} + \frac{1}{15} - \frac{1}{6} > 0
\end{aligned}$$

From above discussion, we get a contradiction which completes the proof. □

Theorem 7 *Let G be a bicyclic graph of order $n \geq 4$, then $H(G) \leq H(B'_n) = H(B_n) = \frac{n}{2} - \frac{1}{15}$ with equality if and only if $G \cong B_n$ or B'_n.*

Proof: It is easy to prove that the theorem holds for $n = 4, 5$. Now we assume $n \geq 6$. Clearly, $H(B'_n) = H(B_n) = \frac{n}{2} - \frac{1}{15}$. Suppose for a contradiction that there is a bicyclic graph $G \neq B_n$ and $G \neq B'_n$ has the maximum value of the harmonic index.

Case 1. There is no pendent vertex in G.

Note that, all the non-isomorphic bicyclic graphs with no pendent vertex has been shown in Figure 2. They are $B_n, B'_n, Y_n, Y'_n, Y''_n$. By calculating the values of harmonic index, we have $H(Y_n) - H(B_n) < 0$, $H(Y'_n) - H(B_n) < 0$, $H(Y''_n) - H(B_n) < 0$. These contradict to the choice of G.

Case 2. There is only one pendent vertex in G, say u.

Subcase 1. The degree of the support vertex of u is two.

Let w be the first vertex with $d(w) \geq 3$ on the path which starts from u. Assume $N(w) = \{v, x, x_1, x_2, \cdots, x_{(d(w)-2)}\}$, $d(v) = 2$. Then $G' := G - wx + ux$. We can get a new graph G'. Therefore we have

$$\begin{aligned}
&H(G') - H(G)\\
=\ & \frac{2}{d(w)+1} + \frac{2}{d(x)+2} + \sum_{i=1}^{d(w)-2} \frac{2}{d(w)-1+d(x_i)}\\
&+\frac{2}{2+2} - \frac{2}{d(w)+2} - \frac{2}{d(w)+d(x)}\\
&- \sum_{i=1}^{d(w)-2} \frac{2}{d(w)+d(x_i)} - \frac{2}{2+1}\\
=\ & \frac{2d(w)-4}{(d(w)+d(x))(d(x)+2)} + \frac{2}{(d(w)+1)(d(w)+2)}\\
&+ \sum_{i=1}^{d(w)-2} \frac{2}{(d(w)-1+d(x_i))(d(w)+d(x_i))} - \frac{1}{6}.
\end{aligned}$$

Note that $3 \leq d(w) \leq 5$, for bicyclic graph G with only one pendent vertex. Then $2 \leq d(x), d(x_i) \leq 4$. It is not difficult to prove that $H(G') - H(G) > 0$, for all the possible values of $d(w), d(x), d(x_i)$. Therefore, this contradicts to the choice of G.

Subcase 2. The degree of the support vertex of u is at least 3.

Let w be the support vertex of u. Note that $3 \leq d(w) \leq 5$, for bicyclic graph G with only one pendent vertex. Suppose $N(w) \setminus \{u\} = \{x, x_1, x_2, \cdots, x_{(d(w)-2)}\}$, $2 \leq d(x), d(x_i) \leq 4$. Then $G' := G - wx + ux$. we can get a new graph G'. Similar to subcase 1, we have

$$\begin{aligned}
&H(G) - H(G')\\
&= \frac{2}{d(w)+1} + \frac{2}{d(x)+2} - \frac{2}{d(w)+2}\\
&+ \sum_{i=1}^{d(w)-2} \frac{2}{d(w)-1+d(x_i)} - \frac{2}{d(w)+1}\\
&- \sum_{i=1}^{d(w)-2} \frac{2}{d(w)+d(x_i)}\\
=\ & \frac{4-2d(w)}{(d(w)+d(x))(d(x)+2)} - \frac{2}{d(w)+1}\\
&- \sum_{i=1}^{d(w)-2} \frac{2}{(d(w)-1+d(x_i))(d(w)+d(x_i))}\\
<\ & 0
\end{aligned}$$

This contradicts to the choice of G.

Case 3. There is at least two pendent vertices in G, say s and t.

Let u be a vertex with maximum degree, and v be a neighbor of u with $d(v) = \max\{d(v_i), v_i \in N(u)\}$. Let $G' := G - uv + st$. If G' is connected, then by Lemma 2, we can get a new graph G' that $H(G') - H(G) > 0$. This contradicts to the choice of G. So we conclude that $G - uv$ is disconnected and has two components G_1 and G_2, and $u \in G_1$, $v \in G_2$. Moreover, one of G_1 and G_2 has no pendent vertex. Note that we take no account of u and v when consider the pendent vertex of G_1 and G_2.

Subcase 1. G_2 has no pendent vertex.

Then G_1 has at least a pendent vertex t. Let s be the support vertex of t. We do not exclude the possibility that $s = u$. Suppose $V(G_1) = n_1$, $E(G_1) = m_1$, $V(G_2) = n_2$, $E(G_2) = m_2$. Then we have $n_1 + n_2 = n, m_1 + m_2 = n$.

Since G_2 has no pendent vertex. Then G_2 is not a tree. So $m_2 \geq n_2$. On the other hand, G_2 have at most two cycles, for G is a bicyclic graph. So $m_2 \leq n_2 + 1$. Then we have either (a) $m_2 = n_2$, and $m_1 = n_1$, or (b)$m_2 = n_2 + 1$, and $m_1 = n_1 - 1$. Now we deduce that

(a)G_1 is a unicyclic graph with at least a pendent vertex, whereas G_2 is also a unicyclic graph with no pendent vertex. So $d_G(v) = 3$, if v is a vertex of cycle; while $d_G(v) = 2$, if v is a pendent vertex of G_2.

(b)G_1 is a tree, whereas G_2 is bicyclic graph with no pendent vertex. So $2 \leq d_G(v) \leq 5$ for G_2 has two cycles;

Let $G' := G - uv + tv$. Suppose $N(u) \setminus \{v\} = \{x_i, 1 \leq i \leq d(u) - 1\}$. Similar to Theorem 6, we have

$$\begin{aligned} & H(G') - H(G) \\ & \geq \frac{2d(u)-4}{(d(v)+2)(d(u)+d(v))} \\ & + \frac{2d(u)-2}{(d(u)-1+d(v))((d(u)+d(v))} - \frac{1}{6} \end{aligned}$$

for (a) $d_G(u) \geq 3$, $d_G(v) = 2$ or $d_G(v) = 3$, we get $H(G') - H(G) > 0$. for (b) $d_G(u) \geq d_G(v)$, $2 \leq d_G(v) \leq 5$, $H(G') - H(G) > 0$. We get the contradiction.

Subcase 2. G_1 has no pendent vertex.

Then G_2 has at least a pendent vertex t. Let s be the support vertex of t. We do not exclude the possibility that $s = v$. Similar to the discussion in subcase 1, since G_1 has no pendent vertex. Then G_1 is not a tree. So $m_1 \geq n_1$. On the other hand, G_1 has at most two cycle, for G is a bicyclic graph. So $m_1 \leq n_1 + 1$. Then we have either (a)$m_1 = n_1$, and $m_2 = n_2$, or (b)$m_1 = n_1 + 1$, and $m_2 = n_2 - 1$.

(a) Therefore G_1 is a cycle, whereas G_2 is also a unicyclic graph. Let w be a neighbor of u. Then $d(u) = 3$, and $d(w) = 2$. Let $G' := G - uw + tw$. Similar to Theorem 6, we get $H(G') - H(G) > 0$.

(b) G_1 is a bicyclic graph, whereas G_2 is tree. G_1 has at least one vertex w meets $d_G(w) = 2$. Let $G' := G - uv + tw$, $d_G(u) \geq 3$, $d_G(w) = 2$, $d_G(v), d_G(s) \leq d_G(u)$. $N(u) \setminus \{v\} = \{x_i, 1 \leq i \leq d(u)-1\}$. $N(v) \setminus \{u\} = \{y_i, 1 \leq i \leq d(v)-1\}$. $N(w) = \{z_i, 1 \leq i \leq 2\}$.

$$\begin{aligned} & H(G') - H(G) \\ = & \sum_{i=1}^{d(u)-1} \left(\frac{2}{d(u)-1+d(x_i)} - \frac{2}{d(u)+d(x_i)}\right) \\ & + \sum_{i=1}^{d(v)-1} \left(\frac{2}{d(v)-1+d(y_i)} - \frac{2}{d(v)+d(y_i)}\right) \\ & + \sum_{i=1}^{2} \left(\frac{2}{3+d(z_i)} - \frac{2}{2+d(z_i)}\right) + \frac{2}{3+2} \\ & - \frac{2}{d(v)+d(u)} + \frac{2}{d(s)+2} - \frac{2}{d(s)+1} \\ \geq & \frac{2d(u)+2d(v)-4}{(d(u)-1+d(v))((d(u)+d(v))} + \frac{2}{5} \\ & - \frac{4}{(d(u)+2)(d(u)+3)} - \frac{2}{d(v)+d(u)} \\ & - \frac{2}{(d(s)+1)(d(s)+2)} \\ \geq & \frac{7}{30} - \frac{4}{(d(u)+2)(d(u)+3)} \\ & - \frac{2}{(d(u)-1+d(v))((d(u)+d(v))} > 0 \end{aligned}$$

From above cases, we get $H(G') - H(G) > 0$, this contradicts to the choice of G. This completes the proof of the theorem. □

5 Further discussion about the connected graphs with maximum harmonic index

In this section, we give a discussion about the connected graphs with maximum harmonic index from a new perspective.

An edge of G, connecting a vertex of degree i and a vertex of degree j, will be called an (i, j)-edge. An (i, j)-edge is symmetric if $i = j$, otherwise it is said to be asymmetric.

Denote by x_{ij} the number of (i, j)-edge, n_i the number of vertices with degree i. The maximum possible vertex degree is $n - 1$. Then we have

$$\sum_{i=1}^{n-1} n_i = n. \sum_{j=1, j\neq i}^{n-1} x_{ij} + 2x_{ii} = in_i. \tag{1}$$

From Eq.(1) we have

$$n_i = \frac{1}{i}\left(\sum_{j=1, j\neq i}^{n-1} x_{ij} + 2x_{ii}\right) \tag{2}$$

Substituting Eq.(2) back into Eq.(1), we get

$$n = \sum_{i=1}^{n-1} \frac{1}{i}\left(\sum_{j=1, j\neq i}^{n-1} x_{ij} + 2x_{ii}\right) \tag{3}$$

Now,

$$\begin{aligned} H(G) &= \sum_{1\leq i\leq j\leq n}^{n-1} \tfrac{2x_{ij}}{i+j} = \sum_{1\leq i<j\leq n}^{n-1} \tfrac{2x_{ij}}{i+j} + \sum_{i=1}^{n-1} \tfrac{x_{ij}}{i} \\ &= \tfrac{n}{2} - \tfrac{1}{2} \sum_{1\leq i<j\leq n}^{n-1} \left(\tfrac{4x_{ij}}{i+j} - \tfrac{x_{ij}}{i} - \tfrac{x_{ij}}{j}\right) \\ &= \tfrac{n}{2} - \tfrac{1}{2} \sum_{1\leq i<j\leq n}^{n-1} \tfrac{(i-j)^2}{ij(i+j)} x_{ij} \\ &= \tfrac{n}{2} - \tfrac{1}{2} \sum_{e\in E(G)} w^*(e) \end{aligned}$$

In the equation $w^*(e)$ is the weight of edge e. If the edge e is symmetric ,then $w^*(e)$ is 0, otherwise $w^*(e) > 0$. To maximize the $H(G)$ value, the number of asymmetric edges need to be as less as possible, and the weight $w^*(e)$ of asymmetric edges need to be as small as possible, i.e. the values of $|i - j|$ are as small as possible.

Since pendent edge is obvious the asymmetric edge. If G reaches the maximum $H(G)$ value, it should has a minimum number of pendent edges. That is why the path P_n has the maximum $H(G)$ value among all the trees with n vertices.

If G is a regular graph, then all edges of G are symmetric. So the regular graphs have the maximum $H(G)$ value among all the graphs with n vertices. And it is easy to deduce that the almost regular graph has the maximum $H(G)$ value among all the graphs with n vertices and m edges. For it has the most symmetric edges and the smallest value of $|i-j|$ for asymmetric edge.

6 Conclusion

In this paper we introduce operations and derived formulas for the harmonic index under these operations. Then we explore the brief proof of the theorem in [30] that the path P_n has the maximum harmonic index. Also we consider the unicyclic and bicyclic graphs, and show the sharp lower and upper bound on the harmonic index of unicyclic and bicyclic graphs. The corresponding graphs which reach the bounds are given.

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