Filomat 36:1 (2022), 125–140
https://doi.org/10.2298/FIL2201125A

Published by Faculty of Sciences and Mathematics,
University of Niš, Serbia
Available at: http://www.pmf.ni.ac.rs/filomat

The Minimum Harmonic Index for Bicyclic Graphs with Given Diameter

Adeleh Abdolghafourian[a], Mohammad A. Iranmanesh[a]

[a]*Department of Mathematical Science, Yazd University, 89195-741 Yazd, I. R. Iran*

Abstract. The harmonic index of a graph G, is defined as the sum of weights $\frac{2}{d(u)+d(v)}$ of all edges uv of G, where $d(u)$ is the degree of the vertex u in G. In this paper we find the minimum harmonic index of bicyclic graph of order n and diameter d. We also characterized all bicyclic graphs reaching the minimum bound.

1. Introduction

Let G be a connected simple graph with vertex set $V(G)$ and edge set $E(G)$. The graph G is said of order n, where $|V(G)| = n$. The degree of a vertex $u \in V(G)$ is denoted by $d_G(u)$ (or simply $d(u)$). Also $N_G(u)$ (or simply $N(u)$) is the set of neighbors of u in G and $N[u] = N(u) \cup \{u\}$. For $u, v \in V(G)$, $d(u, v)$ is the distance between u and v in G and $\mathrm{diam}(G) = \max\{d(u, v); u, v \in G\}$ is the diameter of G. If $X \subseteq G$, then $G - X$ is the graph obtained from G by deleting the vertices of X. Recall that a graph G is called unicyclic, if it contains only one cycle. In this case, $|E(G)| = |V(G)|$. Also a graph G is called a quasi-tree graph, if G is not a tree and there exists $v \in V(G)$, such that $G - v$ is a tree. A bicyclic graph G is a graph with exactly two cycles. In this case $|E(G)| = |V(G)| + 1$. The other notations used here are common and may be found in [11].

The harmonic index of a graph G, is defined as $H(G) = \sum_{uv\in E(G)} \frac{2}{d(u)+d(v)}$. This index first appeared in connection with some conjectures, generated by the computer program Graffiti, [6] and can be viewed as a particular case of the general sum-connectivity index, $\chi_\alpha = \sum_{uv\in E(G)} (d(u) + d(v))^\alpha$, proposed by Zhou and Trinajstić [16] ($H = 2\chi_{-1}$). Du and Zhou [5] studied the sum-connectivity of bicyclic graphs. Also several studies have focused on extremal sum-connectivity index of bicyclic graphs. See for example [2, 4, 10]. We refer the interested readers to [3] for a recent survey about the harmonic index.

Zhong [12] and Zhong and Ciu [14] determined the minimum and maximum harmonic indices for simple connected graphs, trees, unicyclic and characterized the corresponding extremal graphs. Liu [9], showed that if T be a tree of order $n \geq 4$ and diameter d, then $H(T) \geq d + \frac{5}{6} - \frac{n}{2}$. Jerline and Michaelraj [8], proved that for a unicyclic graph G of order $n \geq 7$ and diameter d, $H(G) \geq d + \frac{5}{3} - \frac{n}{2}$.

In [7] the minimum and maximum harmonic indices for caterpillars with diameter 4 are computed. It is also showed that $H(G) \geq d + \frac{5}{3} - \frac{n}{2}$, where G is a quasi-tree graph of order $n \geq 4$ and diameter d, except when $G = U^{1,1}_{5,3}$ or $U^{1,1}_{6,4}$ which are shown in Figure 1 [1].

2020 *Mathematics Subject Classification*. Primary: 05C50; Secondary: 05C09, 05C35
Keywords. Harmonic index, bicyclic graph, diameter
Received: 14 January 2021; Revised: 02 May 2021; Accepted: 31 May 2021
Communicated by Ljubiša D.R. Kočinac
Email addresses: abdolghafourian@yazd.ac.ir (Adeleh Abdolghafourian), iranmanesh@yazd.ac.ir (Mohammad A. Iranmanesh)

This paper is a contribution to the study of harmonic index of simple connected graphs of diameter d and the main purpose is to find a lower bound for harmonic index of bicyclic graphs with respect to their diameters. Indeed all bicyclic graphs reaching the minimum bound are characterized. Let

$$\mathfrak{B}(n,d) = \begin{cases} \frac{16}{15} + \frac{4}{n} + \frac{2}{n+2} + \frac{2(n-5)}{n-1} & d = 3 \\ \frac{7}{5} + \frac{6}{n-1} + \frac{2(n-6)}{n-2} & d = 4 \\ \frac{d-5}{2} + 2 + \frac{6}{n-d+3} + \frac{2(n-d-2)}{n-d+2} & d \geq 5 \end{cases}.$$

We show that $H(G) \geq \mathfrak{B}(n,d)$, where G is a bicyclic graph of order n and diameter d.

In Section 2, we prove the lemmas that will be used in Section 3, where we prove the main theorems.

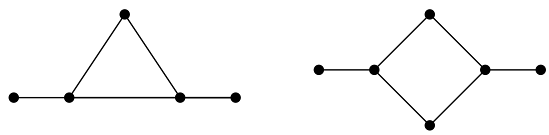
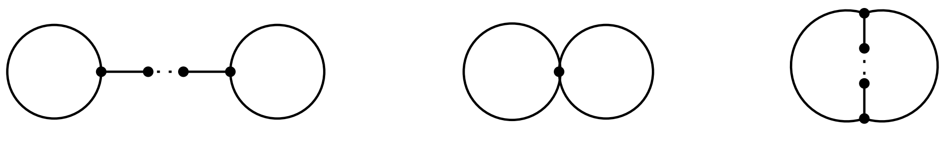


Figure 1: The graphs $U_{5,3}^{1,1}$ (left) and $U_{6,4}^{1,1}$ (right).

2. Preliminaries

Zhong [15], introduced five families of bicyclic graphs of order n with no pendant vertex. We introduce a similar structure as follows.

Let $\mathcal{B}$ be the set of connected bicyclic graphs without pendant vertices. Let $\mathcal{B}^1$ be the set of bicyclic graphs obtained by joining two vertices of disjoint cycles by a path, $\mathcal{B}^2$ be the set of bicyclic graphs obtained by identifying a vertex of each two disjoint cycles and then attaching them. and $\mathcal{B}^3$ be the set of bicyclic graphs obtained from a cycle by adding a path. Obviously, $\mathcal{B} = \mathcal{B}^1 \cup \mathcal{B}^2 \cup \mathcal{B}^3$. For example, the graph $\widetilde{B}_i \in \mathcal{B}^i$, for $i = 1, 2, 3$ is shown in Figure 2.



$\widetilde{B}^1$ $\widetilde{B}^2$ $\widetilde{B}^3$

Figure 2: Bicyclic graphs with no pendant vertex.

For $n \geq 4$, let $\mathcal{B}(n,d)$ be the set of connected bicyclic graphs of order n and diameter d. Every graph $G \in \mathcal{B}(n,d)$ is obtained by attaching some trees to some vertices of a graph $\mathcal{G} \in \mathcal{B}$. We say $\mathcal{G}$ is the root of G. Note that every graph $G \in \mathcal{B}(n,d)$ has a unique root, however it is possible that some non isomorphic bicyclic graphs have common root.

Lemma 2.1. ([13, Lemma 1]) *Let G be a nontrivial connected graph, and let $uv \in E(G)$ be such that $d(u), d(v) \geq 2$ and $N(u) \cap N(v) = \emptyset$. Let G' be the graph obtained from G by contracting the edge uv into a new vertex w and adding a new pendant edge ww' to w. Then $H(G) > H(G')$.*

Corollary 2.2. *If $G \in \mathcal{B}(n,d)$ has minimum harmonic index and $P = u_1 - u_2 - \cdots - u_{d+1}$ is a diametrical path of G, then* *(i) If u_1 is not a pendant vertex, then it is a vertex of a triangle. Similar argument is true for u_{d+1}.*

(ii) Every non pendant vertex of $G-P$ is a vertex of a cycle.

(iii) If C is a cycle of G such that $E(C)\cap E(P)=\emptyset$, then C is a triangle.

Proof. This is an immediate consequence of Lemma 2.1. □

Lemma 2.3. *Let G be a connected graph and $u,v\in V(G)$, such that $2\le d(v)\le d(u)$. Let G_1 obtained from G by attaching two paths of length $r\ge 1$ and $s\ge 1$ to u and v respectively and G_2 obtained from G by attaching one pendant vertex and a path of length $r+s-1$ to u and v respectively. Then $H(G_1)\ge H(G_2)$.*

Proof. If $r=1$, then $G_1=G_2$. Hence assume $r\ge 2$. Assume first that $u\neq v$ and u and v are not adjacent. In the rest of paper, set $z_x=d_G(x)+d_G(u)$ and $w_y=d_G(y)+d_G(v)$. So

$$\begin{aligned}H(G_1)=&H(G)-\sum_{x\in N_G(u)}\frac{2}{z_x(z_x+1)}-\sum_{y\in N_G(v)}\frac{2}{w_y(w_y+1)}\\&+\frac{2}{d(u)+3}+\frac{2}{3}+(r-2)\frac{2}{4}+\begin{cases}\frac{2}{d(v)+2} & s=1\\ \frac{2}{d(v)+3}+\frac{2}{3}+(s-2)\frac{2}{4} & s\ge 2\end{cases},\end{aligned}$$

and

$$H(G_2)=H(G)-\sum_{x\in N_G(u)}\frac{2}{z_x(z_x+1)}-\sum_{y\in N_G(v)}\frac{2}{w_y(w_y+1)}+\frac{2}{d(u)+2}+\frac{2}{d(v)+3}+\frac{2}{3}+(r+s-3)\frac{2}{4}.$$

Hence

$$H(G_1)-H(G_2)=-\frac{2}{(d(u)+3)(d(u)+2)}+\frac{1}{2}+\begin{cases}\frac{2}{(d(v)+2)(d(v)+3)}-\frac{1}{2} & s=1\\ -\frac{1}{3} & s\ge 2\end{cases}.$$

Since $2\le d(v)\le d(u)$, then $H(G_1)\ge H(G_2)$.

Next assume $u\neq v$ and u and v are adjacent. Therefore

$$\begin{aligned}H(G_1)=&H(G)-\sum_{\substack{x\in N_G(u)\\ x\neq v}}\frac{2}{z_x(z_x+1)}-\sum_{\substack{y\in N_G(v)\\ y\neq u}}\frac{2}{w_y(w_y+1)}-\frac{4}{(d(u)+d(v))(d(u)+d(v)+2)}\\&+\frac{2}{d(u)+3}+\frac{2}{3}+\frac{r-2}{2}+\begin{cases}\frac{2}{d(v)+2} & s=1\\ \frac{2}{d(v)+3}+\frac{2}{3}+\frac{s-2}{2} & s\ge 2\end{cases}\end{aligned}$$

and

$$\begin{aligned}H(G_2)=&H(G)-\sum_{\substack{x\in N_G(u)\\ x\neq v}}\frac{2}{z_x(z_x+1)}-\sum_{\substack{y\in N_G(v)\\ y\neq u}}\frac{2}{w_y(w_y+1)}\\&-\frac{4}{(d(u)+d(v))(d(u)+d(v)+2)}+\frac{2}{d(u)+2}+\frac{2}{d(v)+3}+\frac{2}{3}+(r+s-3)\frac{2}{4}.\end{aligned}$$

So $H(G_1)\ge H(G_2)$.

Finally assume $u=v$. In this case without lose of generality, one may assume that $s\ge 2$. Hence

$$H(G_1)=H(G)-\sum_{x\in N_G(u)}\frac{4}{z_x(z_x+2)}+2\left(\frac{2}{d(u)+4}\right)+2\left(\frac{2}{3}\right)+\frac{r+s-4}{2}.$$

and

$$H(G_2) = H(G) - \sum_{x\in N_G(u)} \frac{4}{z_x(z_x+2)} + \frac{2}{d(u)+3} + \frac{2}{d(u)+4} + \frac{2}{3} + \frac{r+s-3}{2}.$$

Hence

$$H(G_1) - H(G_2) = \frac{1}{6} - \frac{2}{(d(u)+3)(d(u)+4)} > 0.$$

This complete the proof. □

Lemma 2.4. *Let $\Gamma_1 \neq G \in \mathcal{B}(n,d)$ with only one pendant vertex u, such that $\mathcal{G} \in \mathcal{B}^1$. If $G - u \in \mathcal{B}(n-1,d-1)$, then there exists $G' \in \mathcal{B}(n,d)$ such that $\mathcal{G}' \in \mathcal{B}^2$ and $H(G) \geq H(G')$.*

Proof. Suppose $u', v' \in V(\mathcal{G})$ are two vertices of degree 3. Let $P' : u' = u'_1 - \cdots - u'_{k+1} = v'$ is the path between u' and v' in $\mathcal{G}$, where $k \geq 1$.

Since deleting u decrease the diameter, one may assume that either $P' \subset P$ or $E(P') \cap E(P) = \emptyset$. If there exists a diametrical path P in G such that $E(P') \cap E(P) = \emptyset$, then Lemma 2.1 implies that there exists $G' \in \mathcal{B}(n,d)$ such that $\mathcal{G}' \in \mathcal{B}^2$ and $H(G) \geq H(G')$.

If every diametrical path of G contains P', then fix a diametrical path $P : u_1 - \cdots - u_{d+1} = u$. Without lose of generality suppose $d(u',u) < d(v',u)$. Note that, in this case, at most one vertex of $N_G(u')$ is of degree 3, otherwise G has two pendant vertices. Also all neighbors of v' are of degree 2.

Let G' obtain from G by contracting the path P' into a new vertex w and adding a new vertex u'_{k+2} such that $V(G') = V(G) \cup \{w, u'_{k+2}\} - \{u'_1, u'_{k+1}\}$ and

$$\begin{aligned} E(G') = {} & E(G) \cup \{uu'_2, u'_k u'_{k+2}\} \cup \{wx : x \in N(u') \cup N(v'), x \neq u'_2, u'_k\} \\ & - \{u'x : x \in N(u')\} - \{v'y : y \in N(v')\}. \end{aligned}$$

Since deleting u from G decrease the diameter, then $u \notin N_G(u')$. Two possibilities are as follows:

(1) $d_G(u') = d_G(v') = 3$. In this case,

$$\begin{aligned} H(G') &= H(G) - \frac{2}{(d(u_d)+1)(d(u_d)+2)} - \sum_{\substack{x\in N_G(u') \\ x\neq u'_2}} \frac{2}{(3+d(x))(4+d(x))} - \sum_{\substack{y\in N(v') \\ y\neq u'_k}} \frac{2}{(3+d(y))(4+d(y))} + A \\ &= H(G) - \frac{1}{5} - \frac{2}{(d(u_d)+1)(d(u_d)+2)} - \frac{2}{(3+d(x))(4+d(x))} + A, \end{aligned}$$

where $A = \frac{1}{3}$ if $k = 1$ and $A = \frac{11}{30}$ if $k \geq 2$. Note that $x \in N_G(u')$ and $d(x) \leq 3$.
The last expression is greater than $H(G)$ if and only if $k \geq 2$ and $d(u_d) = d(x) = 3$. So $G = \Gamma_1$, shown in Figure 3.

(2) $d_G(u') = 4$ and $d_G(v') = 3$. Since $\mathrm{diam}(G - u) < \mathrm{diam}(G)$, then $d(u',u) > 1$ and hence $d(u_d) = 2$ and $d_G(x) = 2$ for every $x \in N(u') - u'_2$. So

$$\begin{aligned} H(G') &= H(G) - \frac{2}{(d(u_d)+1)(d(u_d)+2)} - \sum_{\substack{x\in N(u') \\ x\neq u'_2}} \frac{2}{(4+d(x))(5+d(x))} - \sum_{\substack{y\in N(v') \\ y\neq u'_k}} \frac{4}{(5+d(y))(3+d(y))} + A \\ &= H(G) - \frac{13}{42} - \frac{8}{35} + A < H(G), \end{aligned}$$

where $A = \frac{3}{14}$ if $k = 1$ and $A = \frac{4}{15}$ if $k \geq 2$.

□

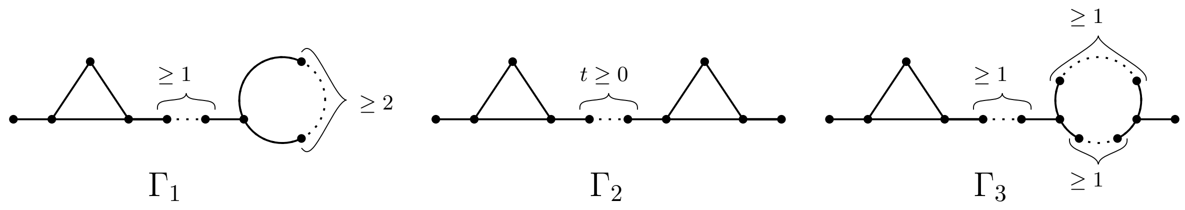


Figure 3: The bicyclic graphs related to Lemmas 2.5, 2.4.

Lemma 2.5. *Let $\Gamma_i \neq G \in \mathcal{B}(n,d)$, $i = 2,3$ (see Figure 3) such that $\mathcal{G} \in \mathcal{B}^1$ and G has only two pendant vertices u, v. If $G-u, G-v \in \mathcal{B}(n-1, d-1)$, then there exists $G' \in \mathcal{B}(n,d)$ such that $\mathcal{G}' \in \mathcal{B}^2$ and $H(G) \geq H(G')$.*

Proof. Suppose $u', v' \in V(\mathcal{G})$ are two vertices of degree 3. Let $P' : u' = u'_1 - \cdots - u'_{k+1} = v'$ is the path between u' and v' in $\mathcal{G}$. Since deleting every pendant vertex decrease the diameter, one may assume that either $P' \subset P$ or $E(P') \cap E(P) = \emptyset$. If there exists a diametrical path P in G such that $E(P') \cap E(P) = \emptyset$, then Lemma 2.1 implies that there exists $G' \in \mathcal{B}(n,d)$ such that $\mathcal{G}' \in \mathcal{B}^2$ and $H(G) \geq H(G')$.

If every diametrical path of G contains P', then fix a diametrical path $P : u = u_1 - \cdots - u_{d+1} = v$. Let G' obtain from G by contracting the path P' into a new vertex w and adding a new vertex u'_{k+2} such that $V(G') = V(G) \cup \{w, u'_{k+2}\} - \{u'_1, u'_{k+1}\}$ and

$$\begin{aligned} E(G') = E(G) &\cup \{uu'_2, u'_k u'_{k+2}\} \cup \{wx : x \in N(u') \cup N(v'), x \neq u'_2, u'_k\} \\ &- \{u'x : x \in N(u')\} - \{v'y : y \in N(v')\}. \end{aligned}$$

Since deleting u, v from G decrease the diameter, then $u, v \notin N_G(u') \cup N_G(v')$. So three cases will arise as follows.

(1) $d_G(u') = d_G(v') = 3$. Note that in this case, at most one vertex of $N_G(u') - \{u'_2\}$ is of degree 3, otherwise $P' \not\subset P$. The same argument is valid for $N_G(v') - u'_k$. Without lose of generality suppose $d_G(u_d) \leq d_G(u_2)$. Hence

$$\begin{aligned} H(G') &= H(G) - \frac{2}{(d(u_d)+1)(d(u_d)+2)} \sum_{\substack{x \in N_G(u') \\ x \neq u'_2}} \frac{2}{(3+d(x))(4+d(x))} - \sum_{\substack{y \in N_G(v') \\ y \neq u'_k}} \frac{2}{(3+d(y))(4+d(y))} + A \\ &= H(G) - \frac{2}{(d(u_d)+1)(d(u_d)+2)} - \frac{2}{(3+d(x))(4+d(x))} - \frac{2}{(3+d(y))(4+d(y))} - \frac{2}{15} + A, \end{aligned}$$

where $A = \frac{1}{3}$ if $k = 1$ and $A = \frac{11}{30}$ if $k \geq 2$.
If $d(u_d) = d(x) = d(y) = 3$, then $H(G') > H(G)$ and $G = \Gamma_2$. Also if $k \geq 2$ and without lose of generality $d(u_d) = d(x) = 3, d(y) = 2$, then $H(G') > H(G)$ and $G = \Gamma_3$. For other possibilities of d_u, d_x and d_y, $H(G') < H(G)$.

(2) $d_G(u') = 3$ and $d_G(v') = 4$. (The case $d_G(u') = 3$ and $d_G(v') = 4$ is similar.) Without lose of generality, suppose $d(v', u_{d+1}) < d(u', u_{d+1})$. Since $\mathrm{diam}(G - u_{d+1}) < \mathrm{diam}(G)$, then $d(v', u_{d+1}) > 1$ and hence $d(u_d) = 2$. Also at most one vertex of $N(u') - u'_2$ is of degree 3, otherwise $P' \not\subset P$ and $d(y) = 2$ for every $y \in N(v') - u'_k$. So

$$\begin{aligned} H(G') &= H(G) - \sum_{\substack{x \in N(u') \\ x \neq u'_2}} \frac{4}{(3+d(x))(5+d(x))} - \sum_{\substack{y \in N(v') \\ y \neq u'_k}} \frac{2}{(4+d(y))(5+d(y))} \\ &\leq H(G) - \frac{4}{35} - \frac{4}{48} - \frac{6}{42} + A < H(G), \end{aligned}$$

where $A = \frac{3}{14}$ if $k = 1$ and $A = \frac{4}{15}$, if $k \geq 2$.

(3) $d_G(u') = d_G(v') = 4$. In this case, since $\mathrm{diam}(G-u'), \mathrm{diam}(G-v') < \mathrm{diam}(G)$, then $d(u', u_1), d(v', u_{d+1}) \geq 2$ and $d(x) = d(y) = 2$ for every $x \in N(u') - u'_2$ and $y \in N(v') - u'_k$. Hence

$$H(G') = H(G) - \sum_{\substack{x\in N(u')\\ x\neq v'}} \frac{4}{(4+d(x))(6+d(x))} - \sum_{\substack{y\in N(v')\\ y\neq u'}} \frac{4}{(4+d(y))(6+d(y))} + A$$
$$= H(G) - 3(\frac{4}{48}) - 3(\frac{4}{48}) + A < H(G),$$

where $A = \frac{1}{4}$ if $k = 1$ and $A = \frac{1}{3}$, if $k \geq 2$.
□

Let K_4^- be a graph obtained from K_4 by deleting an edge. Suppose $\mathrm{B}_{n,2}$ is a bicyclic graph of order n and diameter 2, obtained by attaching $n-4$ pendant vertices to a vertex of degree 3 of K_4^-. Also let $\mathrm{B}^1_{n,3}$ be a bicyclic graph of order n and diameter 3, obtained by attaching a pendant vertex to the vertex of degree 3 of $\mathrm{B}_{n,2}$. Let C_4^+ be the graph obtained from C_4 by adding a new vertex connected to two non adjacent vertices of C_4. For $d \geq 3$ let $\mathrm{B}_{n,d}$ be a bicyclic graph of order n and diameter d, obtained by attaching $n-d-2$ pendant vertices and a path of length $d-3$ to two vertices of degree 3 of C_4^+ (see Figure 4).

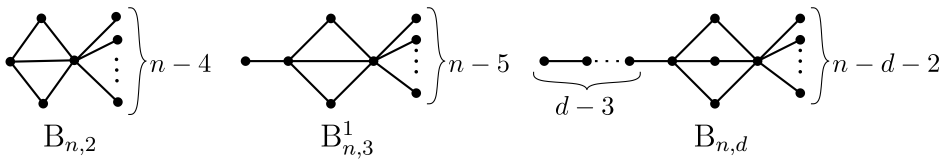


Figure 4: Minimal bicyclic graphs of order n and diameter d.

Zhong and Xu [15], showed that $H(\mathrm{B}_{n,2}) = \frac{4}{5} + \frac{4}{n+1} + \frac{2}{n+2} + \frac{2(n-4)}{n}$ is the minimum harmonic index in the set of harmonic indices of bicyclic graphs of order n. So $H(G) \geq H(\mathrm{B}_{n,2})$ for every $G \in \mathcal{B}(n,2)$ and equality holds if and only if $G = \mathrm{B}_{n,2}$. We claim that if $d = 3$, then $H(G) > H(\mathrm{B}^1_{n,3}) = \frac{7}{5} + \frac{6}{n-1} + \frac{2(n-6)}{n-2}$ for every $\mathrm{B}^1_{n,3} \neq G \in \mathcal{B}(n,3)$ and if $d \geq 4$, then $H(G) > H(\mathrm{B}_{n,d}) = \frac{d-5}{2} + 2 + \frac{6}{n-d+3} + \frac{2(n-d-2)}{n-d+2}$ for every $\mathrm{B}_{n,d} \neq G \in \mathcal{B}(n,d)$. For $3 \leq d \leq n-2$, define the two variable function $\mathfrak{B}(n,d)$ as follows.

$$\mathfrak{B}(n,d) = \begin{cases} \frac{16}{15} + \frac{4}{n} + \frac{2}{n+2} + \frac{2(n-5)}{n-1} & d = 3 \\ \frac{7}{5} + \frac{6}{n-1} + \frac{2(n-6)}{n-2} & d = 4 \\ \frac{d-5}{2} + 2 + \frac{6}{n-d+3} + \frac{2(n-d-2)}{n-d+2} & d \geq 5 \end{cases}$$

Lemma 2.6. *Let $f_1(x) = \frac{x}{2} - \mathfrak{B}(x,3)$, $f_2(x) = \frac{x}{2} - \mathfrak{B}(x,4)$ and $f_3(x) = \frac{x}{2} - \frac{6}{x+3} - \frac{2(x-2)}{x+2} + \frac{1}{2}$. Then $f_1(x) \geq \frac{73}{210}$ is an increasing function for $x \geq 5$, $f_2(x) \geq \frac{2}{5}$ is an increasing function when $x \geq 6$ and $f_3(x) \geq \frac{3}{5}$ is an increasing function when $x \geq 3$.*

Proof. It is easy to see that $f_1'(x) = \frac{1}{2} + \frac{4}{x^2} + \frac{2}{(x+2)^2} - \frac{8}{(x-1)^2}$. So if $x \geq 5$, then $x-1 \geq 4$ and $\frac{1}{2} - \frac{8}{(x-1)^2} \geq \frac{1}{2} - \frac{8}{16} = 0$. Hence $f_1'(x) > 0$, when $x \geq 5$ and $f_1(x) \geq f_1(5) = \frac{73}{210}$ is an increasing function.

Also if $x \geq 6$, then $f_2'(x) = \frac{1}{2} + \frac{6}{(x-1)^2} - \frac{8}{(x-2)^2} \geq \frac{1}{2} + + \frac{6}{(x-1)^2} - \frac{8}{16} > 0$. So $f_2(x) \geq f_2(6) = \frac{2}{5}$ is an increasing function when $x \geq 6$.

Suppose $x \geq 3$, then $f_3'(x) = \frac{1}{2} + \frac{6}{(x+3)^2} - \frac{8}{(x+2)^2} \geq \frac{1}{2} + \frac{6}{(x+3)^2} - \frac{8}{25} > 0$. Therefore $f_3(x) \geq f_3(3) = \frac{3}{5}$ is an increasing function too. □

3. Main results

In this section we show that $H(G) \geq \mathfrak{B}(n,d)$ for every $G \in \mathcal{B}(n,d)$, where $d \geq 3$.

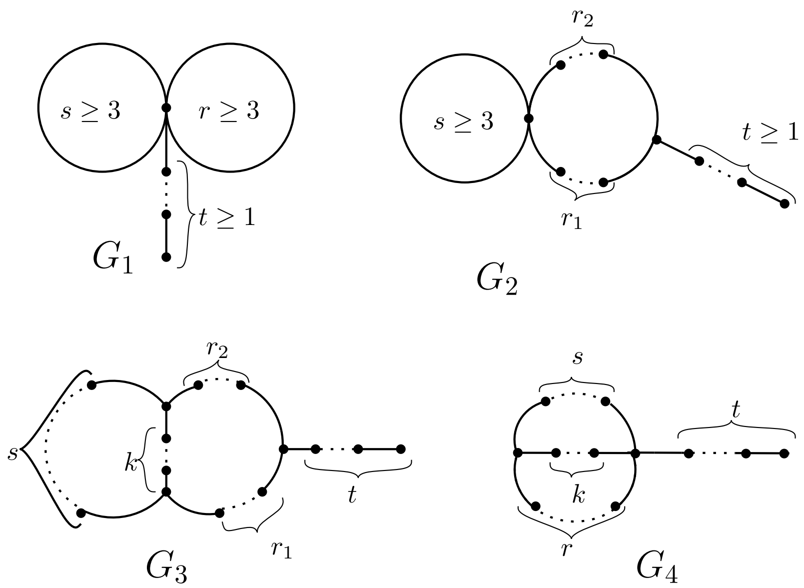


Figure 5: The graphs related to Lemma 3.1.

Lemma 3.1. *Let $G \in \mathcal{B}(n,d)$, $n-d \geq 3$ and $d \geq 3$, such that G has at least one pendant vertex. If for every pendant vertex $w \in G$, $G - w \in \mathcal{B}(n-1,d-1)$ then $H(G) \geq \mathfrak{B}(n,d)$. The equality holds if and only if $G = \mathrm{B}^1_{6,3}$ or $\mathrm{B}_{7,4}$.*

Proof. Let $\mathcal{G}$ be the root of G. If G has more than two pendant vertices, then there is a pendant vertex v such that $G - v \in \mathcal{B}(n-1,d)$, a contradiction. So G has at most two pendant vertices.

- If G has one pendant vertex w, then two cases will arise as follows.

(1) $\mathcal{G} \in \mathcal{B}^1 \cup \mathcal{B}^2$. By Lemma 2.4, without lose of generality, assume $G = \Gamma_1$ or $\mathcal{G} \in \mathcal{B}^2$. So if $G = \Gamma_1$, then $d \geq 5$, $n-d \geq 3$ and $H(\Gamma_1) = \frac{n}{2} - \frac{4}{15}$. Therefore

$$H(\Gamma_1) - \mathfrak{B}(n,d) = \frac{n-d}{2} - \frac{6}{n-d+3} - \frac{2(n-d-2)}{n-d+2} + \frac{1}{2} - \frac{4}{15} > 0,$$

by Lemma 2.6. If $\mathcal{G} \in \mathcal{B}^2$, then $\mathcal{G}$ is obtained by attaching two disjoint cycles of lengths r, $s \geq 3$, joining together in vertex u. So $|V(\mathcal{G})| = r+s-1$, $d_{\mathcal{G}}(u) = 4$ and the other vertices of $\mathcal{G}$ are of degree 2. Hence G is obtained by attaching a path of length t either to u or to a vertex of degree 2. Hence $G = G_1$ or $G = G_2$, the graphs shown in Figure 5.
Suppose $G = G_1$. Since $\mathrm{diam}(G-w) < \mathrm{diam}(G)$, we find that $t \geq 2$, $n \geq 7$ and $H(G) = \frac{n}{2} - \frac{17}{42}$. So if $d = 3$, then $r = s = 3$, $t = 2$ and $n = 7$. Hence $H(G) = \frac{65}{21} > \frac{796}{315} = \mathfrak{B}(7,3)$. If $d = 4$, then $n \geq 8$ and $H(G) - \mathfrak{B}(n,4) = \frac{n}{2} - \frac{6}{n-1} - \frac{2(n-6)}{n-2} - \frac{7}{5} - \frac{17}{42} > 0$, by Lemma 2.6. If $d \geq 5$, then $n-d \geq 4$ and $H(G) - \mathfrak{B}(n,d) = \frac{n-d}{2} - \frac{6}{n-d+3} - \frac{2(n-d-2)}{n-d+2} + \frac{1}{2} - \frac{17}{42} > 0$, by Lemma 2.6.
Suppose $G = G_2$ and without lose of generality, $r_1 \leq r_2$. If $r_1 = 0$, then $H(G) = \frac{n}{2} - \frac{11}{35} + A$, where $A = 0$ if $t = 1$ and $A = \frac{1}{15}$ if $t \geq 2$. Also if $r_1 \geq 1$, then $H(G) = \frac{n}{2} - \frac{11}{30} + A$, where $A = 0$ if $t = 1$ and $A = \frac{1}{15}$ if $t \geq 2$. So if $d = 3$, then $t = 1$, $r_1 = 0$ and $n \geq 6$. Therefore $H(G) - \mathfrak{B}(n,3) \geq \frac{n}{2} - \frac{4}{n} - \frac{2}{n+2} - \frac{2(n-5)}{n-1} - \frac{145}{105} > 0$, by Lemma 2.6. If $d = 4$, then $n \geq 7$ and $H(G) \geq \frac{n}{2} - \frac{11}{30}$. Therefore $H(G) - \mathfrak{B}(n,4) = \frac{n}{2} - \frac{6}{n-1} - \frac{2(n-6)}{n-2} - \frac{53}{30} > 0$, by Lemma 2.6. Also if $d \geq 5$, then $H(G) \geq \frac{n}{2} - \frac{11}{30}$ and $H(G) - \mathfrak{B}(n,d) = \frac{n-d}{2} - \frac{6}{n-d+3} - \frac{2(n-d-2)}{n-d+2} + \frac{2}{15} > 0$, by Lemma 2.6.

(2) $\mathcal{G} \in \mathcal{B}_3$. In this case, G is obtained by attaching a path of length $t \geq 1$, to either a vertex of degree 2 or a vertex of degree 3 of $\mathcal{G}$. So $G = G_3$ or G_4, shown in Figure 5. Without lose of generality, suppose if $G = G_3$, then $r_1, r_2, k \geq 0$, $r_1 \leq r_2$. Also if $G = G_4$, then $k \leq r, s$ and $r, s, t \geq 1$. The following possibilities will arise.

(*i*) $k = 0$. Hence

$$H(G_3) = \frac{n}{2} - \frac{13}{15} + A + \begin{cases} \frac{2}{3} & r_1 = r_2 = 0 \\ \frac{19}{30} & r_1 = 0,\ r_2 \geq 1 \\ \frac{3}{5} & r_1, r_2 \geq 1 \end{cases},$$

where $A = 0$, if $t = 1$ and $A = \frac{1}{15}$, otherwise.

If $d = 3$, then $t = 1$, $r_1 = 0$ and $n \geq 5$. So $H(G_3) - \mathfrak{B}(n,3) \geq \frac{n}{2} - \frac{4}{n} - \frac{2}{n+2} - \frac{2(n-5)}{n-1} - \frac{7}{30} - \frac{16}{15} > 0$, by Lemma 2.6. If $d = 4$, then either $r_1 = 0$ and $t \geq 2$ or $r_1 \geq 1$. Therefore if $r_1 = 0$, then $n \geq 6$ and $H(G_3) \geq \frac{n}{2} - \frac{1}{6}$. Hence $H(G_3) - \mathfrak{B}(n,4) \geq \frac{6}{2} - \frac{1}{6} - \mathfrak{B}(6,4) > 0$, by Lemma 2.6. Also if $r_1 \geq 1$ then $n \geq 7$ and $H(G_3) \geq \frac{n}{2} - \frac{4}{15}$. So $H(G_3) - \mathfrak{B}(n,4) \geq \frac{7}{2} - \frac{4}{15} - \mathfrak{B}(7,4) > 0$, by Lemma 2.6. If $d \geq 5$, then $H(G_3) - \mathfrak{B}(n,d) \geq \frac{n-d}{2} - \frac{6}{n-d+3} - \frac{2(n-d-2)}{n-d+2} + \frac{1}{2} - \frac{4}{15} > 0$.

Also $H(G_4) = \frac{n}{2} + A$, where $A = -\frac{73}{210}$ if $t = 1$ and $A = -\frac{26}{105}$ if $t \geq 2$. So if $d = 3$, then $n \geq 6$ and $H(G_4) - \mathfrak{B}(n,3) \geq \frac{n}{2} - \frac{4}{n} - \frac{2}{n+2} - \frac{2(n-5)}{n-1} - \frac{16}{15} - \frac{73}{210} > 0$, by Lemma 2.6. If $d = 4$, then $n \geq 7$ and $H(G_4) - \mathfrak{B}(n,4) \geq \frac{n}{2} - \frac{6}{n-1} - \frac{2(n-6)}{n-2} - \frac{7}{5} - \frac{73}{210} > 0$. Also if $d \geq 5$ then $H(G_4) - \mathfrak{B}(n,d) \geq \frac{n-d}{2} - \frac{6}{n-d+3} - \frac{2(n-d-2)}{n-d+2} + \frac{1}{2} - \frac{73}{210} > 0$.

(*ii*) $k \geq 1$. So

$$H(G_3) = \frac{n}{2} - \frac{9}{10} + A + \begin{cases} \frac{2}{3} & r_1 = r_2 = 0 \\ \frac{19}{30} & r_1 = 0,\ r_2 \geq 1 \\ \frac{3}{5} & r_1, r_2 \geq 1 \end{cases},$$

· where $A = 0$, if $t = 1$ and $A = \frac{1}{15}$, otherwise. If $d = 3$, then $r_1 = 0$, $t = 1$ and $n \geq 6$. Therefore

$$H(G_3) - \mathfrak{B}(n,3) \geq \frac{n}{2} - \frac{4}{n} - \frac{2}{n+2} - \frac{2(n-5)}{n-1} - \frac{4}{3} > 0.$$

If $d = 4$, then $n \geq 7$ and $H(G_3) - \mathfrak{B}(n,4) \geq \frac{n}{2} - \frac{6}{n-1} - \frac{2(n-6)}{n-2} - \frac{17}{10} > 0$. Also if $d \geq 5$ then $H(G_3) - \mathfrak{B}(n,d) \geq \frac{n-d}{2} - \frac{6}{n-d+3} - \frac{2(n-d-2)}{n-d+2} + \frac{1}{5} > 0$.

Also $H(G_4) = \frac{n}{2} + A$, where $A = -\frac{2}{5}$ if $t = 1$ and $A = -\frac{3}{10}$ if $t \geq 2$. So if $d = 3$, then $t = 1$ and $H(G_4) - \mathfrak{B}(n,3) \geq \frac{n}{2} - \frac{4}{n} - \frac{2}{n+2} - \frac{2(n-5)}{n-1} - \frac{22}{15} > 0$. If $d = 4$, then $H(G_4) - \mathfrak{B}(n,4) \geq \frac{n}{2} - \frac{6}{n-1} - \frac{2(n-6)}{n-2} - \frac{9}{5} > 0$. Also if $d \geq 5$ then $H(G_4) - \mathfrak{B}(n,d) \geq \frac{n-d}{2} - \frac{6}{n-d+3} - \frac{2(n-d-2)}{n-d+2} + \frac{1}{10} > 0$.

- If G has two pendant vertices, then by Lemma 2.5, without lose of generality, suppose either $\mathcal{G} \in \mathcal{B}_2 \cup \mathcal{B}_3$ or $G = \Gamma_i$, $i = 2, 3$. If $\mathcal{G} \in \mathcal{B}_2 \cup \mathcal{B}_3$, then Lemma 2.3 implies that without lose of generality, one may assume that G is obtained by attaching a pendant vertex w and a path of length t to two vertices u and v of $\mathcal{G}$, respectively, such that $d(v) \leq d(u)$. So there are four cases as follows.

(1) $\mathcal{G} \in \mathcal{B}^2$. Suppose $|V(\mathcal{G})| = m$, then $n = m + t + 1$ and $H(\mathcal{G}) = \frac{m}{2} - \frac{1}{6}$. Since only one vertex of $\mathcal{G}$ is of degree 4 and the other vertices are of degree 2, then either $d_G(u) = d_G(v) = 3$ or $d_G(u) = 5$, $d_G(v) = 3$. Note that since deleting every pendant vertex, decrease the diameter, then $u \neq v$ and $d \geq 4$. Hence two possibilities will arise as follows.

(*i*) $u \notin N(v)$. Hence

$$H(G) = H(\mathcal{G}) - \sum_{x \in N_{\mathcal{G}}(u)} \frac{2}{(z_x - 1)z_x} - \sum_{y \in N_{\mathcal{G}}(v)} \frac{2}{(w_y - 1)w_y} + \frac{2}{d(u)+1} + \begin{cases} \frac{2}{d(v)+1} & t = 1 \\ \frac{2}{d(v)+2} + \frac{2}{3} + \frac{t-2}{2} & t \geq 2 \end{cases}.$$

If $d(u) = d(v) = 3$, then

$$H(G) \geq \frac{n}{2} - \frac{17}{30} + \begin{cases} 0 & t = 1 \\ \frac{1}{15} & t \geq 2 \end{cases}.$$

Hence by Lemma 2.6, if $d = 4$ then $n \geq 7$ and $H(G) - \mathfrak{B}(n,4) \geq \frac{n}{2} - \frac{6}{n-1} - \frac{2(n-6)}{n-2} - \frac{59}{30} > 0$. Also if $d \geq 5$, then $n \geq 8$ and $n - d \geq 3$. So $H(G) - \mathfrak{B}(n,d) \geq \frac{n-d}{2} - \frac{6}{n-d+3} - \frac{2(n-d-2)}{n-d+2} - \frac{1}{15} > 0$.
If $d(u) = 5$ and $d(v) = 3$ then

$$H(G) \geq \frac{n}{2} - \frac{76}{105} + \begin{cases} 0 & t = 1 \\ \frac{1}{15} & t \geq 2 \end{cases}.$$

Since u, v are not adjacent, there exists a cycle of length at least 4 in G. So by Lemma 2.6, if $d = 4$, then $n \geq 8$ and $H(G) - \mathfrak{B}(n,4) \geq \frac{n}{2} - \frac{6}{n-1} - \frac{2(n-6)}{n-2} - \frac{223}{105} > 0$. Also if $d \geq 5$, then $n \geq 9$ and $n - d \geq 4$. Therefore $H(G) - \mathfrak{B}(n,d) \geq \frac{n-d}{2} - \frac{6}{n-d+3} - \frac{2(n-d-2)}{n-d+2} - \frac{47}{210} > 0$.

(*ii*) $u \in N(v)$. In this case

$$H(G) = H(\mathcal{G}) - \sum_{\substack{x \in N_{\mathcal{G}}(u) \\ x \neq v}} \frac{2}{(z_x - 1)z_x} - \sum_{\substack{y \in N_{\mathcal{G}}(v) \\ y \neq u}} \frac{2}{(w_y - 1)w_y} + \frac{2}{d(u)+1} - \frac{4}{(d(u)+d(v)-2)(d(u)+d(v))}$$
$$+ \begin{cases} \frac{2}{d(v)+1} & t = 1 \\ \frac{2}{d(v)+2} + \frac{2}{3} + \frac{t-2}{2} & t \geq 2 \end{cases}.$$

By the same calculation as **(*i*)**, one may easily see that $H(G) > \mathfrak{B}(n,d)$.

(2) $\mathcal{G} \in \mathcal{B}^3$ and $d_{\mathcal{G}}(u', v') = 1$, where u', v' are two vertices of degree 3 in $\mathcal{G}$. Suppose $|V(\mathcal{G})| = m$, then $n = m + t + 1$ and $H(\mathcal{G}) = \frac{m}{2} - \frac{1}{15}$. Note that if $u = v$ then $\mathrm{diam}(G - w) = \mathrm{diam}(G)$, a contradiction. So $u \neq v$ and $d \geq 3$. Hence either $d_G(u) = d_G(v) = 3$ or $d_G(u) = 4$, $d_G(v) = 3$ or $d_G(u) = d_G(v) = 4$. Therefore two possibilities will arise as follows.

(*i*) $u \notin N(v)$. Then $d \geq 4$ and

$$H(G) = H(\mathcal{G}) - \sum_{x \in N_{\mathcal{G}}(u)} \frac{2}{(z_x - 1)z_x} - \sum_{y \in N_{\mathcal{G}}(v)} \frac{2}{(w_y - 1)w_y} + \frac{2}{d(u)+1} + \begin{cases} \frac{2}{d(v)+1} & t = 1 \\ \frac{2}{d(v)+2} + \frac{2}{3} + \frac{t-2}{2} & t \geq 2 \end{cases}.$$

If $d(u) = d(v) = 3$ then since $n - d \geq 3$, then $n \geq 7$ and

$$H(G) \geq \frac{n}{2} - \frac{7}{15} + \begin{cases} 0 & t = 1 \\ \frac{1}{5} & t \geq 2 \end{cases}.$$

If $d = 4$, then $H(G) - \mathfrak{B}(n,4) = \frac{n}{2} - \frac{6}{n-1} - \frac{2(n-6)}{n-2} - \frac{28}{15} > 0$. Also if $d \geq 5$, then $H(G) - \mathfrak{B}(n,d) \geq \frac{n-d}{2} - \frac{6}{n-d+3} - \frac{2(n-d-2)}{n-d+2} + \frac{1}{30} > 0$, by Lemma 2.6.
If $d(u) = 4$ and $d(v) = 3$ then u has at least one neighbor of degree 3 and

$$H(G) \geq \frac{n}{2} - \frac{23}{42} + \begin{cases} 0 & t = 1 \\ \frac{1}{15} & t \geq 2 \end{cases}.$$

If $d = 4$, then $n \geq 7$ and $H(G) - \mathfrak{B}(n,4) \geq \frac{n}{2} - \frac{6}{n-1} - \frac{2(n-6)}{n-2} - \frac{409}{210} > 0$. Also if $d \geq 5$ and $t \geq 2$, then $H(G) - \mathfrak{B}(n,d) \geq \frac{n-d}{2} - \frac{6}{n-d+3} - \frac{2(n-d-2)}{n-d+2} - \frac{1}{21} > 0$.
Note that since $u \notin N(v)$, then both $d(u)$ and $d(v)$ are not equal to 4.

(*ii*) $u \in N(v)$. Then $d \geq 3$ and

$$H(G) = H(\mathcal{G}) - \sum_{\substack{x \in N_{\mathcal{G}}(u) \\ x \neq v}} \frac{2}{(z_x - 1)z_x} - \sum_{\substack{y \in N_{\mathcal{G}}(v) \\ y \neq u}} \frac{2}{(w_y - 1)w_y} + \frac{2}{d(u)+1} - \frac{4}{(d(u)+d(v)-2)(d(u)+d(v))}$$
$$+ \begin{cases} \frac{2}{d(v)+1} & t = 1 \\ \frac{2}{d(v)+2} + \frac{2}{3} + \frac{t-2}{2} & t \geq 2 \end{cases}.$$

If $d = 3$ then since deleting every pendant vertices decrease the diameter, then $d(u) = d(v) = 4$ and $n = 6$. So $G = \mathrm{B}^1_{6,3}$. If $d \geq 4$, then by the same calculation as **(*i*)**, one may easily see that $H(G) > \mathfrak{B}(n, d)$.

(3) $\mathcal{G} \in \mathcal{B}^3$ and $d_{\mathcal{G}}(u', v') > 1$, where u', v' are two vertices of degree 3 in $\mathcal{G}$. Suppose $|V(\mathcal{G})| = m$, then $n = m + t + 1$ and $H(\mathcal{G}) = \frac{m}{2} - \frac{1}{10}$. So either $d(u) = d(v) = 3$ or $d(u) = 4$, $d(v) = 3$ or $d(u) = d(v) = 4$. Note that if $u = v$ or $u \in N(v)$ then $\mathrm{diam}(G - w) = \mathrm{diam}(G)$, a contradiction. Therefore $u \neq v$ and u, v are not adjacent. Hence $d \geq 4$ and

$$H(G) = H(\mathcal{G}) - \sum_{x \in N_{\mathcal{G}}(u)} \frac{2}{(z_x - 1)z_x} - \sum_{y \in N_{\mathcal{G}}(v)} \frac{2}{(w_y - 1)w_y} + \frac{2}{d(u)+1} + \begin{cases} \frac{2}{d(v)+1} & t = 1 \\ \frac{2}{d(v)+2} + \frac{2}{3} + \frac{t-2}{2} & t \geq 2 \end{cases}.$$

If $d(u) = d(v) = 3$ then

$$H(G) \geq \frac{n}{2} - \frac{1}{2} + \begin{cases} 0 & t = 1 \\ \frac{1}{15} & t \geq 2 \end{cases}.$$

If $d = 4$, then $n \geq 7$ and $H(G) - \mathfrak{B}(n, 4) \geq \frac{n}{2} - \frac{6}{n-1} - \frac{2(n-6)}{n-2} - \frac{19}{10} > 0$. Also if $d \geq 5$, then $H(G) - \mathfrak{B}(n, d) \geq \frac{n-d}{2} - \frac{6}{n-d+3} - \frac{2(n-d-2)}{n-d+2} > 0$.
If $d(u) = 4$ and $d(v) = 3$ then

$$H(G) \geq \frac{n}{2} - \frac{3}{5} + \begin{cases} 0 & t = 1 \\ \frac{1}{15} & t \geq 2 \end{cases}.$$

If $d = 4$, then $n \geq 8$ and $H(G) - \mathfrak{B}(n, 4) \geq \frac{n}{2} - \frac{6}{n-1} - \frac{2(n-6)}{n-2} - 2 > 0$. Also if $d \geq 5$, then $n \geq 9$ and $n - d \geq 4$. So $H(G) - \mathfrak{B}(n, d) \geq \frac{n-d}{2} - \frac{6}{n-d+3} - \frac{2(n-d-2)}{n-d+2} - \frac{1}{10} > 0$.
If $d(u) = d(v) = 4$, then

$$H(G) = \frac{n}{2} - \frac{3}{5} - \begin{cases} \frac{1}{10} & t = 1 \\ 0 & t \geq 2 \end{cases}.$$

If $d = 4$, then $t = 1$ and $n \geq 7$. If $n = 7$, then $G = \mathrm{B}_{7,4}$ and $H(G) = \mathfrak{B}(7, 4)$. If $n \geq 8$, then $H(G) - \mathfrak{B}(n, 4) = \frac{n}{2} - \frac{6}{n-1} - \frac{2(n-6)}{n-2} - \frac{21}{10} > 0$. Also if $d \geq 5$, then $n \geq 8$. If $n - d = 3$, then $t \geq 2$. So $G = \mathrm{B}_{n,d}$ and $H(G) = \mathfrak{B}(n, d)$. If $n - d \geq 4$, then $H(G) - \mathfrak{B}(n, d) \geq \frac{n-d}{2} - \frac{6}{n-d+3} - \frac{2(n-d-2)}{n-d+2} - \frac{2}{10} > 0$.

(4) $G = \Gamma_i$, $i = 2, 3$. So $d \geq 5$.
If $G = \Gamma_2$, then $d \geq 5$, $n - d = 3$ and $H(G) = \frac{n}{2} - A$, where $A = \frac{2}{5}$ if $t = 0$ and $A = \frac{13}{30}$ if $t = 0$. Therefore $H(G) - \mathfrak{B}(n, d) = \frac{3}{5} - A > 0$. If $G = \Gamma_3$, then $H(G) = \frac{n}{2} - \frac{7}{15}$. So $H(G) - \mathfrak{B}(n, d) = \frac{n-d}{2} - \frac{6}{n-d+3} - \frac{2(n-d-2)}{n-d+2} + \frac{1}{30} > 0$.
□

Theorem 3.2. *Let $G \in \mathcal{B}(n, d)$ and $d \geq 3$ then $H(G) \geq \mathfrak{B}(n, d)$ and equality holds if and only if $G = \mathrm{B}^1_{n,3}$, where $d = 3$ and $G = \mathrm{B}_{n,d}$, where $d \geq 4$.*

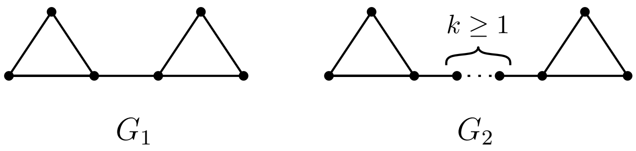


Figure 6: The graphs related to Theorem 3.2

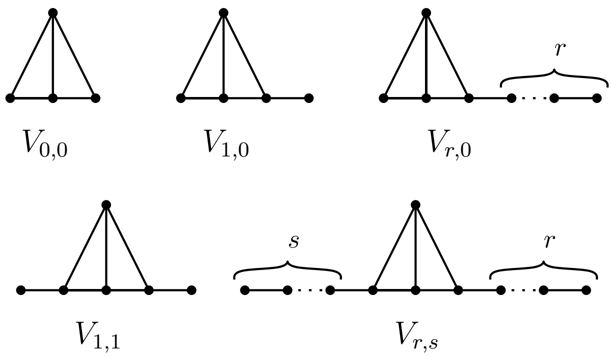


Figure 7: Bicyclic graph of order n and diameter d, such that $n - d = 2$.

Proof. By induction on n. First suppose $n - d = 2$. So if $P \subset G$ be a diametrical path, then only one vertex of G is not in P. Note that two cycles of G should have a common vertex not in P and all other vertices of G should be in P, since every cycle has at least one vertex which is not in P. Therefore $\mathcal{G} \in \mathcal{B}^3$ and $G = V_{r,s}$, is a quasi-tree graph introduced in [1]. The graph $V_{r,s}$ obtained by adding two paths of lengths r, s to two vertices of degree 2 of K_4^-, (see Figure 7). The authors showed [1], $H(V_{r,s}) \geq d + \frac{5}{3} - \frac{n}{2}$, where equality holds if and only if $r = s = 1$. One may easily see that if $d \leq 5$, then $d + \frac{5}{3} - \frac{n}{2} > \mathfrak{B}(n, d)$, since $n - d = 2$. Suppose $d \geq 5$. Then $G = V_{s,r}$ where $r, s \geq 0$ and $r + s \geq 3$. Hence by [1, Table 1], $H(G) \geq \frac{d}{2} + \frac{11}{15} > \mathfrak{B}(d + 2, d)$.

Suppose $n - d = 3$. So two vertices of G are not in its diametrical path. If G has no pendant vertex, then Corollary 2.2 implies that every cycle of G is a triangle. Hence G is one of the graph shown in Figure 6, since $d \geq 3$. By an easy calculation, it is seen that $H(G_1) = \frac{44}{15} > \mathfrak{B}(6, 3)$, $H(G_2) = \frac{29}{10} + \frac{k}{2} > \mathfrak{B}(k + 6, k + 3)$.

Assume G has at least one pendant vertex. If for every pendant vertex of G, namely v, $\text{diam}(G - v) < \text{diam}(G)$, then Lemma 3.1 implies that $H(G) > \mathfrak{B}(n, d)$. Hence suppose there exists a pendant vertex $v \in G$ such that $\text{diam}(G - v) = \text{diam}(G)$ and $N_G(v) = u$. Since v is a pendant vertex, $G - v \in \mathcal{B}(n - 1, d)$ and $G - v$ is one of the graph shown in Figure 7. Now by [1], $H(G - v) \geq d + \frac{5}{3} - \frac{(n-1)}{2} = \frac{d}{2} + \frac{2}{3}$, where equality holds if and only if $G - v = V_{1,1}$. Also $2 \leq d_{G-v}(u) \leq 3$ and

$$H(G) = H(G - v) + \frac{2}{d_{G-v}(u) + 2} - \sum_{x \in N_{G-v}(u)} \frac{2}{(d_{G-v}(x) + d_{G-v}(u))(d_{G-v}(x) + d_{G-v}(u) + 1)}$$

Note that at most one neighbor of u is of degree one. If $d_{G-v}(u) = 2$ then $d \geq 4$ and $G - v \neq V_{1,1}$. Therefore $H(G - v) > \frac{d}{2} + \frac{2}{3}$. If $d = 4$, then $n = 7$ and $H(G) > \frac{87}{30} > \frac{14}{5} = \mathfrak{B}(7, 4)$. If $d \geq 5$, then

$$H(G) - \mathfrak{B}(n, d) \geq H(G - v) + \frac{7}{30} - \mathfrak{B}(n, d) > \frac{d}{2} + \frac{27}{30} - \mathfrak{B}(n, d) = 0$$

Suppose $d_{G-v}(u) = 3$, then at most one neighbor of u is of degree less than 3. So $H(G) \geq H(G - v) + \frac{43}{210}$.

If $d = 3$ then $G - v = V_{1,0}$ and $H(G - v) = \frac{23}{10}$. Hence $H(G) \geq \frac{263}{105} > \frac{143}{60} = \mathfrak{B}(6, 3)$.

If $d = 4$, then $n = 7$ and $H(G - v) \geq \frac{8}{3}$. Hence $H(G) > \mathfrak{B}(7, 4)$.

Also if $d \geq 5$, then $H(G-v) \geq \frac{d}{2} + \frac{11}{15}$. Therefore $H(G) - \mathfrak{B}(d+3,d) \geq 0$.

Suppose $n > d+3$ and for convenience, G has minimum harmonic index among all graphs in $\mathcal{B}(n,d)$. Let $P = v_1 - v_2 - \cdots - v_{d+1}$ is a diametrical path of G. If G has no pendant vertex, then by Corollary 2.2, every cycle of G is a triangle. So at most two vertices of G are not in its diametrical path. Hence $n - d \leq 3$, a contradiction.

Suppose G has at least one pendant vertex. If for every pendant vertex $v \in G$, $G - v \in \mathcal{B}(n-1, d-1)$, then by Lemma 3.1, $H(G) > \mathfrak{B}(n,d)$. Hence assume there exists a pendant vertex v in G such that $G - v \in \mathcal{B}(n-1,d)$ and $N(v) = u$. Note that $d(u) \leq n - d + 1$, since diam(G) $= d$. Suppose there exist k_i vertices of degree i in $N(u)$ for $1 \leq i \leq r$. It is clear that there exists $i > 1$ such that $k_i \neq 0$. Hence

$$\begin{aligned} H(G) &= H(G-v) + \frac{2}{1+d(u)} - \sum_{v \neq x \in N(u)} \frac{2}{(d(u)-1+d(x))(d(u)+d(x))} \\ &= H(G-v) + \frac{2}{1+d(u)} - \frac{2k_1}{d(u)(d(u)+1)} - \cdots - \frac{2k_r}{(d(u)+r-1)(u+r)}. \end{aligned} \tag{1}$$

There are three cases as follows.

(*i*) $d(u) \leq n - d - 1$. In this case, Equation 1, implies that

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

Since the function $f(x) = \frac{2(x+4)}{x(1+x)(2+x)}$ is a decreasing function for $x > 0$, $f(d(u)) \geq f(n-d-1)$. So if $d = 4$, then induction hypothesis implies

$$H(G) \geq \frac{7}{5} + \frac{6}{n-2} + \frac{2(n-7)}{n-3} + \frac{2(n-1)}{(n-5)(n-4)(n-3)}$$

and $H(G) - \mathfrak{B}(n,4) > 0$. Also if $d \geq 5$ then

$$H(G) \geq 2 + \frac{d-5}{2} + \frac{6}{n-d+2} + \frac{2(n-d-3)}{n-d+1} + \frac{2(n-d+3)}{(n-d-1)(n-d)(n-d+1)},$$

and

$$H(G) - \mathfrak{B}(n,d) \geq \frac{12(5(n-d)+3)}{(n-d+2)(n-d+3)(n-d)((n-d)^2-1)} > 0.$$

Suppose $d = 3$ and $d(u) \leq n-5$. To the contrary, suppose there exists only one vertex $x \in N(u)$ such that $d(x) = 2$ and other neighbors of u are pendant vertices. Then if $u = v_1$ or v_4, we find that $d \geq 4$, a contradiction. If $u = v_2$ or v_3, then G is a tree, another contradiction. So $u \neq v_i$ for $1 \leq i \leq 4$. Without lose of generality assume $d(v_1, x) < d(v_4, x) = t$. Then $d(v_4, v) = 1 + d(v_4, u) = 2 + d(v_4, x) = 2 + t \geq 4$, a contradiction. Therefore there exist $x, y \in N(u)$ such that $d(x), d(y) \geq 2$. Hence by Equation 1,

$$\begin{aligned} H(G) &\geq H(G-v) + \frac{2}{1+d(u)} - \frac{2(d(u)-3)}{d(u)(d(u)+1)} - \frac{4}{(d(u)+1)(d(u)+2)} \\ &= H(G-v) + \frac{2(d(u)+6)}{(1+d(u))d(u)(d(u)+2)}. \end{aligned}$$

Since the function $f(x) = \frac{2(x+6)}{(1+x)x(x+2)}$ is a decreasing function,

$$H(G) - \mathfrak{B}(n,3) \geq \frac{12(80+37n^2+78n-66n^3+15n^4)}{n(n-4)(n-5)(n-3)(n^2-1)(n^2-4)} > 0.$$

Assume that $d(u) = n-4$. If at least three neighbors of u, are not pendant vertices, then the Equation 1 implies

$$\begin{aligned} H(G) &\geq H(G-v) + \frac{2}{1+d(u)} - \frac{2(d(u)-4)}{d(u)(d(u)+1)} - \frac{6}{(d(u)+1)(d(u)+2)} \\ &= H(G-v) + \frac{2(d(u)+8)}{(1+d(u))d(u)(d(u)+2)}. \end{aligned}$$

So

$$H(G) - \mathfrak{B}(n,3) \geq \frac{48(3x^3-3x^2-5x-4)}{(x-3)x(x-4)(x^2-1)(x^2-4)} > 0.$$

Also if there exist $x, y \in N(u)$ such that $d(x) \geq 2$ and $d(y) \geq 3$, then

$$\begin{aligned} H(G) &\geq H(G-v) + \frac{2}{1+d(u)} - \frac{2(d(u)-3)}{d(u)(d(u)+1)} - \frac{2}{(d(u)+1)(d(u)+2)} - \frac{2}{(d(u)+2)(d(u)+3)} \\ &= H(G-v) + \frac{2(d(u)+9)}{(d(u)+3)d(u)(d(u)+1)}. \end{aligned}$$

Since $f(x) = \frac{2(x+9)}{(x+3)x(x+1)}$ is an decreasing function,

$$H(G) - \mathfrak{B}(n,3) \geq \frac{12(-16-22n-15n^2+11n^3)}{n(n-4)(n-3)(n^2-1)(n^2-4)} > 0.$$

Suppose there exist $x, y \in N(u)$ such that $d(x) = d(y) = 2$ and $d(z) = 1$ for every vertices $x, y \neq z \in N(u)$. If $u \notin P$, then since every neighbor of G is of degree at most 2, then $N(u) \cap P \subset \{v_1, v_4\}$. Also since $\text{diam}(G) = 3$, then $|N(u) \cap \{v_1, v_4\}| = 1$. So u is adjacent to exactly one vertex of P, since $d(u) = n-4$. without lose of generality suppose $x = v_1 \in N(u)$. Hence $d(v, v_4) \geq 5$, a contradiction.
If $u \in P$ and $u = v_1$, then $d(v, v_4) > 3$, a contradiction. The same argument is valid for v_4. Therefore without lose of generality, suppose $u = v_2$, $x = v_1$, $y = v_3$ and $u \neq z \in N(v_1)$. Hence $N(z) \cap N[u] = v_1$. Hence either z is a pendant vertex or there exists a vertex $w \in N(z)$. If z is a pendant vertex, then $d > 3$, a contradiction. If $w = v_4$, then $d(v_1, v_4) \leq 2$, another contradiction. Also if $w \neq v_4$, then $d(v, t) \geq 4$, which is a contradiction.

(*ii*) $d(u) = n-d$. So either $u = v_i$, where $i \in \{1, d+1\}$ or u is adjacent to at least two vertices of P.
Assume first that $u \in P$. If $u = v_1$ or v_d, then $\text{diam}(G-v) < \text{diam}(G)$, a contradiction. So there is exactly one vertex $w \in G-p$, such that $w \notin N(u)$. If $\sum_{x \in N(u)} d(x) = n-d+1$, then exactly one neighbors of u is of degree 2 and the other neighbors are pendant vertices. Hence without lose of generality, $u = v_2$ and $N(w) = \{v_{k-1}, v_k, v_{k+1}\}$ for $5 \leq k \leq d$, since G is a bicyclic graph. Therefore $d \geq 5$, $n \geq 9$ and G is the graph which is shown in Figure 8. Therefore $H(G) = \frac{d-5}{2} + \frac{2(n-d-1)}{n-d+1} + \frac{2}{n-d+2} + A$, where $A = \frac{11}{5}$ if $t = 0$, and $A = \frac{31}{15}$ if $t = 1$, and $A = \frac{32}{15}$, if $t \geq 2$. Hence

$$H(G) - \mathfrak{B}(n,d) \geq \frac{(n-d)^3 + 6(n-d)^2 + 41(n-d) - 84}{15(n-d+1)(n-d+2)(n-d+3)} > 0.$$

If $\sum_{x \in N(u)} d(x) > n-d+1$.
It is easy to see that if $d \geq 4$ then $H(G) > \mathfrak{B}(n,d)$. Also if $d = 3$ and $\sum_{x \in N(u)} d(x) > n-d+2$, then $H(G) > \mathfrak{B}(n,3)$. Suppose $d = 3$ and $\sum_{x \in N(u)} d(x) = n-d+2$. Hence u has either exactly two neighbors of degree 2 or one neighbor of degree 3. Without lose of generality suppose $u = v_2$. If u has two neighbors of degree 2, namely x, v_3, then $N(w) \subseteq \{x, v_4\}$ and G is unicycle, a contradiction. If $d(v_3) = 3$, then $N(w) \subseteq \{v_3, v_4\}$ and G is unicycle, another contradiction.
Suppose now that $u \notin P$. If $v_1 \in N(u)$ then $v_{d+1} \notin N(u)$, otherwise $\text{diam}(G) = 2$. So there exists a vertex of degree at least 3 and a vertex of degree 2 in $N(u)$. If the other neighbors of u are pendant vertices,

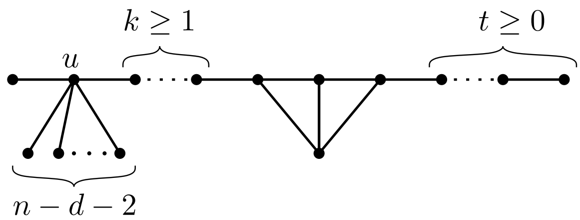


Figure 8: The graph related to Case (*ii*) of Theorem 3.2.

then G is a unicyclic graph, a contradiction. Hence there is another vertex of degree at least 2 in $N(u)$ and hence by Equation 1,

$$\begin{aligned} H(G) &\geq H(G-v) + \frac{2}{1+d(u)} - \frac{2(d(u)-4)}{d(u)(d(u)+1)} - \frac{4}{(d(u)+1)(d(u)+2)} - \frac{2}{(d(u)+2)(d(u)+3)} \\ &= H(G-v) + \frac{2(d(u)^2+13d(u)+24)}{(d(u)+1)d(u)(d(u)+2)(d(u)+3)}. \end{aligned}$$

If $d = 3$, then $d(u) = n-3$ and

$$\begin{aligned} H(G) - \mathfrak{B}(n,3) &\geq \frac{4}{n-1} + \frac{2}{n+1} + \frac{2(n-6)}{n-2} - \frac{4}{n} - \frac{2}{n+2} - \frac{2(n-5)}{n-1} + \frac{2(n^2+7n-6)}{n(n-3)(n-2)(n-1)} \\ &= \frac{12(2+5n+7n^2)}{n(n-3)(n^2-1)(n^2-4)} > 0. \end{aligned}$$

If $d = 4$ then

$$H(G) - \mathfrak{B}(n,4) \geq \frac{8(n+2)}{(n-1)(n-2)(n-3)(n-4)} > 0.$$

If $d \geq 5$ then

$$H(G) - \mathfrak{B}(n,d) \geq \frac{8((n-d)+6)}{(n-d+1)(n-d)(n-d+2)(n-d+3)} > 0.$$

(*iii*) $d(u) = n-d+1$.
If $u \notin P$ then u is adjacent to at least three vertices of P. Since $\text{diam}(G) > 2$, u is not adjacent to both v_1, v_{d+1}. Hence there exist two vertices of degree at least 3 and a vertex of degree at least 2 in $N(u)$. By a similar argument as in Case (*ii*), $H(G) > \mathfrak{B}(n,d)$.
If $u \in P$, then $G - P \subset N(u)$ and $|N(u) \cap P| = 2$. So $u \neq v_1, v_{d+1}$. Suppose $u = v_i$, where $2 \leq i \leq d$ and $x \in N(u) - P$. Then $N(x) \cap P \subseteq \{v_{i-2}, v_{i-1}, v_i, v_{i+1}, v_{i+2}\}$. Also if $v_k, v_{k'} \in N(x)$, then $k - k' \leq 2$. Therefore $|N(x) \cap P| \leq 3$. If $d(x) \geq 4$, then $|N(x) \cap N(u) - P| \geq 1$. So if $d \geq 4$, then u has a neighbor of degree at least 4 and two neighbors of degree at least 2. Therefore Equation 1 implies that $H(G) > \mathfrak{B}(n,d)$. If $d = 3$, then x should be adjacent to at least three neighbors of u and hence u has at least two neighbors of degree at least 2, one neighbor of degree at least 3 and one neighbor of degree at least 4. Therefore Equation 1 implies,

$$\begin{aligned} H(G) &\geq H(G-v) + \frac{2}{1+d(u)} - \frac{4}{(d(u)+1)(d(u)+2)} - \frac{2}{(d(u)+2)(d(u)+3)} - \frac{2}{(d(u)+3)(d(u)+4)} \\ &- \frac{2(d(u)-5)}{d(u)(d(u)+1)} = H(G-v) + \frac{2(d(u)^2+20d(u)+40)}{(d(u)+1)d(u)(d(u)+2)(d(u)+4)} \end{aligned}$$

and

$$H(G) - \mathfrak{B}(n,d) \geq \frac{4(2n-1)}{(n-2)n(n^2-1)} > 0.$$

Suppose $d(x) \leq 3$ for every $x \in N(u) - P$. If $d(x) = 1$ for every $x \in G - P$, then G is a tree, a contradiction. If there exists only one vertex in $G - P$ such that $d(x) = 2$, then G is a unicyclic graph, a contradiction too. So either there is a vertex x in $G - P$ such that $d(x) \geq 3$ or there exist two vertices z, y in $G - P$ such that $\deg(z), d(y) \geq 2$. Since $E(G) = n + 1$, counting the degrees of vertices, implies that either there is a vertex x in $G - P$ such that $d(x) = 3$ and $d(w) = 1$ for every $w \in G - (P \cup N(x))$ or there are two vertices z, y in $G - P$ such that $\deg(z), d(y) = 2$ and $d(w) = 1$ for every $w \in G - (P \cup N(y) \cup N(z))$.
If $u \in P - \{v_2, v_d\}$ then $d \geq 4$ and there exist at least two vertex in $P \cap N(u)$ of degree more than 1 and $H(G) \geq \mathfrak{B}(n,d)$, by a similar argument as in Case (*ii*). Also if $u = v_2$ (or $u = v_d$) and $d(v_1) \geq 2$ (or $d(v_{d+1}) \geq 2$), then there exist at least two vertices in $P \cap N(u)$ of degree more than 1 and $H(G) \geq \mathfrak{B}(n,d)$. So without lose of generality suppose $u = v_2$ and $d(v_1) = 1$. Then u can only have a common neighbor with v_3 or v_4. Hence there are two possibilities.

(*a*) There exists a vertex $x \in N(u) - P$ such that $d(x) = 3$ and $d(w) = 1$ for every $w \in G - (P \cup N(x))$. If $x \in N(v_3) \cap N(v_4)$, then $G = V_{1,r}$, which is shown in Figure 7, and $H(G) > \mathfrak{B}(n,d)$. If $x \in N(v_3)$ and $x \notin N(v_4)$, then u has a neighbor of degree 2 and two neighbors of degree 3. One may easily see that $H(G) > \mathfrak{B}(n,d)$. If $x \notin N(v_3) \cup N(v_4)$, then u has three neighbors of degree 2 and a neighbor of degree 3 and $H(G) > \mathfrak{B}(n,d)$.

(*b*) There exist two vertices z, y in $G - P$ such that $d(z), d(y) = 2$ and $d(w) = 1$ for every $w \in G - (P \cup N(y) \cup N(z))$. If $y, z \in N(v_3)$ and $d = 3$, then $G = B^1_{n,3}$ and $H(G) = \mathfrak{B}(n,3)$. If $y, z \in N(v_3)$ and $d \geq 4$, then

$$\begin{aligned} H(G) &\geq H(G-v) + \frac{2}{1+d(u)} - \frac{2(d(u)-4)}{d(u)(d(u)+1)} - \frac{4}{(d(u)+1)(d(u)+2)} - \frac{2}{(d(u)+3)(d(u)+4)} \\ &= H(G-v) + \frac{2(d(u)^3 + 19d(u)^2 + 78d(u) + 96)}{(1+d(u))(d(u)+2)(d(u)+4)(d(u)+3)d(u)} \end{aligned}$$

and it is easy to see that $H(G) - \mathfrak{B}(n,d) > 0$. If $y, z \in N(v_4)$, then $G = B_{n,d}$. So if $d = 3$ then $G = B_{n,3}$ and $H(G) = 1 + \frac{6}{n} + \frac{2(n-5)}{n-1}$. Hence $H(G) - \mathfrak{B}(n,3) = \frac{4(n^2+2n+15)}{n(n+2)} > 0$. If $d \geq 4$ then $G = B_{n,d}$ and $H(G) = \mathfrak{B}(n,d)$. If $z, y \notin N(v_3) \cup N(v_4)$, then u has at least five neighbors of degree 1 and $H(G) > \mathfrak{B}(n,d)$. If without lose of generality, $y \in N(v_3)$ and $z \notin N(v_3) \cup N(v_4)$, then u has three neighbors of degree 2 and a neighbor of degree 3 and $H(G) > \mathfrak{B}(n,d)$.

Now the proof is complete. □

References

[1] A. Abdolghafourian, M.A. Iranmanesh, On Harmonic index and diameter of quasi-tree graphs, J. Math. 2021 (2021), Article ID 6650407, 9 pages.
[2] N. Akhterm, I. Tomescu, Bycylic graphs with minimum general sum-connectivity index for $-1 \leq \alpha < 0$, Publ. Roman. Acad. A. 16 (2015) 484–489.
[3] A. Ali, L. Zhong, I. Gutman, Harmonic index and its generalizations: extremal results and bounds, MATCH Commun. Math. Comput. Chem. 81 (2019) 249–311.
[4] M. Arshad, I. Tomescu, Maximum general sum-connectivity index with $-1 \leq \alpha < 0$ for bicyclic graphs, Math. Rep. 19 (2017) 93–96.
[5] Z. Du, B. Zhou, On sum-connectivity index of bicyclic graphs, Bull. Malays. Math. Sci. Soc. 35 (2012) 101–117.
[6] S. Fajtlowicz, On conjectures of Graffiti-II, Congr. 60 (1987) 187–197.
[7] M.A. Iranmanesh, M. Saheli, On the harmonic index and harmonic polynomial of Caterpillars with diameter four, Iranian J. Math. Chem. 6 (2015) 35–43.
[8] J.A. Jerline, B.A. Michaelraj, On a conjecture of harmonic index and diameter of graphs, Kragujevac J. Math. 40 (2016) 73–78.
[9] J. Liu, On harmonic index and diameter of graphs, J. Appl. Math. Phys. 1 (2013) 5–6.
[10] I. Tomescu, Extremal results concerning the general sum-connectivity index in some classes of connected graphs, ROMAI J. 10 (2014) 45–51.
[11] D.B. West, Introduction to Graph Theory,(2nd edition), Prentice hall Upper Saddle River, 2001.

[12] L. Zhong, The harmonic index for graphs, Appl. Math. Lett. 25 (2012) 561–566.
[13] L. Zhong, The minimum harmonic index for unicyclic graphs with given diameter, Discuss. Math. Graph Theory 38 (2018) 429–442.
[14] L. Zhong, Q. Cui, The harmonic index for unicyclic graphs with given girth, Filomat 29 (2015) 673–686.
[15] L. Zhong, K. Xu, The harmonic index for bicyclic graphs, Util. Math. 90 (2013) 23–32.
[16] B. Zhou, N. Trinajstić, On general sum-connectivity index, J. Math. Chem. 47 (2010) 210–218.