Filomat 27:1 (2013), 51–55
DOI 10.2298/FIL1301051W

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

A lower bound for the harmonic index of a graph with minimum degree at least two

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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 give 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.

1. Introduction

In this work, we consider the harmonic index. For a simple graph (or a molecular graph) $G = (V, E)$, the harmonic index $H(G)$ is defined in [1] as $H(G) = \sum_{uv\in E(G)} \frac{2}{d(u)+d(v)}$, where $d(u)$ denotes the degree of a vertex u in G. Favaron et al. [2] considered the relation between harmonic index and the eigenvalues of graphs. Zhong [3] found the minimum and maximum values of the harmonic index for simple connected graphs and trees, and characterized the corresponding extremal graphs. Deng, Balachandran, Ayyaswamy, Venkatakrishnan [4] 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 [5], since we always have $H(G) \leq R(G)$ for any graph G. Deng, Tang, Zhang [6] considered the harmonic index $H(G)$ and the radius $r(G)$ and strengthened some results relating the Randić index and the radius in [7] [8] [9]. Deng, Balachandran, Ayyaswamy, Venkatakrishnan [10] determined the trees with the second-the sixth maximum harmonic indices, and unicyclic graphs with the second-the fifth maximum harmonic indices, and bicyclic graphs with the first-the fourth maximum harmonic indices. For other related results see [11] [12] [13] [14]. Here we will establish a best possible lower bound for the harmonic index of a graph, a triangle-free graph, respectively, with n vertices and minimum degree at least two and characterize the extremal graphs.

2. A lower bound for the harmonic index of a graph with minimum degree at least two

In the section, we will establish a best possible lower bound for the harmonic index of a graph with minimum degree at least two and characterize the extremal graphs.

2010 *Mathematics Subject Classification*. Primary 05C07; Secondary 05C15
Keywords. Graph, the harmonic index, the minimum degree
Received: 10 May 2012; Accepted: 26 September 2012
Communicated by Dragan Stevanović
Research supported by Hunan Provincial Natural Science Foundation of China (13JJ3053) and the Program Excellent Talent Hunan Normal University (ET13101)
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For an edge $e = uv$ of a graph G, its weight is defined to be $\frac{2}{d(u)+d(v)}$. The harmonic index of G is the sum of weights over all its edges.

Lemma 2.1. *If e is an edge with maximal weight in G, then $H(G-e) < H(G)$.*

Proof. Let $e = uv$. Since uv is an edge with maximal weight in G, we have $d(w) \geq d(v)$ for $w \in N(u)$ and $d(w) \geq d(u)$ for $w \in N(v)$. Note that $\frac{1}{x} - \frac{1}{x-1}$ is increasing for $x > 1$.

$$\begin{aligned} H(G) - H(G-e) = & \frac{2}{d(u)+d(v)} + \sum_{w \in N(u)\setminus\{v\}} \left(\frac{2}{d(u)+d(w)} - \frac{2}{d(u)+d(w)-1}\right) \\ & + \sum_{w \in N(v)\setminus\{u\}} \left(\frac{2}{d(v)+d(w)} - \frac{2}{d(v)+d(w)-1}\right) \\ \geq & \frac{2}{d(u)+d(v)} + (d(u)-1)\left(\frac{2}{d(u)+d(v)} - \frac{2}{d(u)+d(v)-1}\right) \\ & +(d(v)-1)\left(\frac{2}{d(v)+d(u)} - \frac{2}{d(v)+d(u)-1}\right) \\ = & \frac{2}{d(u)+d(v)-1} - \frac{2}{d(u)+d(v)} > 0 \end{aligned}$$

which proves the result.

Let $K_{a,b}$ be the complete bipartite graph with a and b vertices in its two partite sets, respectively. For $n \geq 4$, let $K^*_{2,n-2}$ be the graph obtained from $K_{2,n-2}$ by joining an edge between the two non-adjacent vertices of degree $n-2$. Obviously, $H(K^*_{2,n-2}) = h_1(n) = 4 + \frac{1}{n-1} - \frac{12}{n+1}$. Let $\delta(G)$ be the minimum degree of the graph G.

Theorem 2.2. *Let G be a graph with $n \geq 3$ vertices and $\delta(G) \geq 2$. Then $H(G) \geq h_1(n)$ with equality if and only if $G = K^*_{2,n-2}$.*

Proof. It is easy to check that the assertion is true for $n = 4$. Suppose it holds for $4 \leq k < n$; we next show that it also holds for n.

Let G be a graph with $n > 4$ vertices. If $\delta(G) \geq 3$, then by Lemma 1, the deletion of an edge with maximal weight yields a graph G' of minimal degree at least two such that $H(G') < H(G)$. So, we only need to prove the result is true for G with $\delta(G) = 2$.

Case 1. Every pair of adjacent vertices of degree two has a common neighbor.

Let u_1 and u_2 be a pair of adjacent vertices with degree two in G which has a common neighbor u_3. Obviously, $2 \leq d(u_3) \leq n-1$.

Subcase 1.1. If $d(u_3) = 2$, let $G_1 = G - \{u_1, u_2, u_3\}$, then $H(G_1) \geq h_1(n-3)$ by the induction hypothesis, and $H(G) = H(G_1) + \frac{3}{2} \geq h_1(n-3) + \frac{3}{2} > h_1(n)$.

Subcase 1.2. If $d(u_3) \geq 4$, let $G_2 = G - \{u_1, u_2\}$, then $H(G_2) \geq h_1(n-2)$ by the induction hypothesis. Note that $\frac{1}{x} - \frac{1}{x-2}$ is increasing for $x > 2$.

$$\begin{aligned} H(G) = & H(G_2) + \frac{1}{2} + \frac{4}{d(u_3)+2} + \sum_{v \in N(u_3)\setminus\{u_1,u_2\}} \left(\frac{2}{d(u_3)+d(v)} - \frac{2}{d(u_3)+d(v)-2}\right) \\ \geq & H(G_2) + \frac{1}{2} + \frac{4}{d(u_3)+2} + (d(u_3)-2)\left(\frac{2}{d(u_3)+2} - \frac{2}{d(u_3)}\right) \\ = & H(G_2) + \frac{1}{2} + \frac{4}{d(u_3)} - \frac{4}{d(u_3)+2} \\ \geq & h_1(n-2) + \frac{1}{2} + \frac{4}{d(u_3)} - \frac{4}{d(u_3)+2} \\ \geq & h_1(n-2) + \frac{1}{2} + \frac{4}{n-1} - \frac{4}{n+1} > h_1(n). \end{aligned}$$

Subcase 1.3. If $d(u_3) = 3$, let u_4 be the neighbor of u_3 in G different from u_1 and u_2, where $2 \leq d(u_4) \leq n-3$.

(i) Suppose that $d(u_4) = 2$. Denote by u_5 the neighbor of u_4 in G different from u_3, where $2 \leq d(u_5) \leq n-4$. Let $G_3 = G - u_4 + u_3u_5$, then $H(G_3) \geq h_1(n-1)$ by the induction hypothesis. Note that $\frac{1}{x} - \frac{1}{x+1}$ is decreasing for $x > 0$.

$$\begin{aligned} H(G) = & H(G_3) + \frac{2}{5} + \frac{2}{d(u_5)+2} - \frac{2}{d(u_5)+3} \\ \geq & H(G_3) + \frac{2}{5} + \frac{2}{n-2} - \frac{2}{n-1} \\ \geq & h_1(n-1) + \frac{2}{5} + \frac{2}{n-2} + \frac{2}{n-1} > h_1(n). \end{aligned}$$

(ii) Suppose that $3 \leq d(u_4) \leq n-3$. Let $G_4 = G - u_1 - u_2 - u_3$, then $H(G_4) \geq h_1(n-3)$ by the induction hypothesis. Note that $\frac{2}{x+2} - \frac{6}{x+1} + \frac{4}{x}$ is decreasing for $x > 0$.

$$\begin{aligned} H(G) = & \ H(G_4) + \tfrac{1}{2} + \tfrac{4}{5} + \tfrac{2}{d(u_4)+3} + \sum_{v \in N(u_4) \setminus \{u_3\}} \left(\tfrac{2}{d(u_4)+d(v)} - \tfrac{2}{d(u_4)+d(v)-1}\right) \\ \geq & \ H(G_4) + \tfrac{13}{10} + \tfrac{2}{d(u_4)+3} + (d(u_4)-1)\left(\tfrac{2}{d(u_3)+2} - \tfrac{2}{d(u_4)+1}\right) \\ = & \ H(G_4) + \tfrac{13}{10} + \tfrac{2}{d(u_4)+3} - \tfrac{6}{d(u_4)+2} + \tfrac{4}{d(u_4)+1} \\ \geq & \ H(G_4) + \tfrac{13}{10} + \tfrac{2}{n} - \tfrac{6}{n-1} + \tfrac{4}{n-2} \\ \geq & \ h_1(n-3) + \tfrac{13}{10} + \tfrac{2}{n} - \tfrac{6}{n-1} + \tfrac{4}{n-2} > h_1(n). \end{aligned}$$

Case 2. There is a pair of adjacent vertices of degree two without common neighbor.

Let u_1 and u_2 be a pair of adjacent vertices with degree two in G which has no common neighbor. Denote by u_3 the neighbor of u_1 in G different from u_2. Let $G_5 = G - u_1 + u_2u_3$, then $H(G_5) \geq h_1(n-1)$ by the induction hypothesis, and $H(G) = H(G_5) + \frac{1}{2} \geq h_1(n-1) + \frac{1}{2} > h_1(n)$.

Case 3. There is no pair of adjacent vertices of degree two.

Let u be a vertex of degree two with neighbors v and w in G.

Subcase 3.1. $vw \notin E$, where $3 \leq d(v) \leq n-2$ and $3 \leq d(w) \leq n-2$. Let $G_6 = G - u + vw$, then $H(G_6) \geq h_1(n-1)$ by the induction hypothesis. Note that $f(x,y) = \frac{2}{x+2} + \frac{2}{y+2} - \frac{2}{x+y} \geq f(n-2, n-2)$ for $3 \leq x \leq n-2$ and $3 \leq y \leq n-2$, since $\frac{\partial f}{\partial x} < 0$ and $\frac{\partial f}{\partial y} < 0$.

$$\begin{aligned} H(G) = & \ H(G_6) + \tfrac{2}{d(v)+2} + \tfrac{2}{d(w)+2} - \tfrac{2}{d(v)+d(w)} \\ \geq & \ H(G_6) + f(n-2, n-2) \\ \geq & \ h_1(n-1) + \tfrac{4}{n} - \tfrac{1}{n-2} > h_1(n). \end{aligned}$$

Subcase 3.2. $vw \in E$, where $3 \leq d(v) \leq n-1$ and $3 \leq d(w) \leq n-1$. Let $G_7 = G - u$, then $H(G_7) \geq h_1(n-1)$ by the induction hypothesis. Note that $g(x,y) = \frac{2}{x+y} + \frac{6}{x+1} + \frac{6}{y+1} - \frac{2}{x+y-2} - \frac{6}{x+2} - \frac{6}{y+2} \geq g(n-1, n-1)$ for $3 \leq x \leq n-1$ and $3 \leq y \leq n-1$, since $\frac{\partial g}{\partial y}(\frac{\partial g}{\partial x}) < 0$ and $\frac{\partial g}{\partial x} \leq \frac{\partial g(x,3)}{\partial x} < 0$, and $\frac{\partial g}{\partial x}(\frac{\partial g}{\partial y}) < 0$ and $\frac{\partial g}{\partial y} \leq \frac{\partial g(3,y)}{\partial y} < 0$.

$$\begin{aligned} H(G) = & \ H(G_7) + \tfrac{2}{d(v)+2} + \tfrac{2}{d(w)+2} - \tfrac{2}{d(v)+d(w)-2} \\ & + \sum_{z \in N(v) \setminus \{u,w\}} \left(\tfrac{2}{d(v)+d(z)} - \tfrac{2}{d(v)+d(z)-1}\right) + \sum_{z \in N(w) \setminus \{u,v\}} \left(\tfrac{2}{d(w)+d(z)} - \tfrac{2}{d(w)+d(z)-1}\right) \\ \geq & \ H(G_7) + \tfrac{2}{d(v)+2} + \tfrac{2}{d(w)+2} - \tfrac{2}{d(v)+d(w)-2} \\ & + (d(v)-2)\left(\tfrac{2}{d(v)+2)} - \tfrac{2}{d(v)+1}\right) + (d(w)-2)\left(\tfrac{2}{d(w)+2} - \tfrac{2}{d(w)+1}\right) \\ & \text{(with equality if and only if } d(z) = 2 \text{ for all } z \in N(v) \cup N(w) \setminus \{u, v, w\}) \\ = & \ H(G_7) + \tfrac{2}{d(v)+d(w)} + \tfrac{6}{d(v)+1} + \tfrac{6}{d(w)+1} - \tfrac{2}{d(v)+d(w)-2)} - \tfrac{6}{d(v)+2}) - \tfrac{6}{d(v)+2} - \tfrac{6}{d(w)+2}) \\ \geq & \ H(G_7) + g(n-1, n-1) \\ & \text{(with equality if and only if } d(v) = d(w) = n-1) \\ \geq & \ h_1(n-1) + \tfrac{1}{n-1} + \tfrac{12}{n} - \tfrac{1}{n-2} - \tfrac{12}{n+1} \\ & \text{(with equality if and only if } G_7 = K^*_{2,n-3}) \\ = & \ h_1(n) \end{aligned}$$

with equality if and only if $G = K^*_{2,n-2}$.

Hence, the assertion is true for all $n \geq 4$.

3. A lower bound for the harmonic index of a triangle-free graph with minimum degree at least two

In the section, we will give a best possible lower bound for the harmonic index of a triangle-free graph with minimum degree at least two and characterize the extremal graphs.

Theorem 3.1. *Let G be a triangle-free graph of order $n \geq 4$ with $\delta(G) \geq 2$. Then $H(G) \geq h_2(n) = 4 - \frac{8}{n}$ with equality if and only if $G = K_{2,n-2}$.*

Proof. It is easy to check that the assertion is true for $n = 4$. Suppose it holds for $4 \le k < n$; we next show that it also holds for n.

Let G be a graph with $n > 4$ vertices. If $\delta(G) \ge 3$, then by Lemma 1, the deletion of an edge with maximal weight yields a graph G' of minimal degree at least two such that $H(G') < H(G)$. So, we only need to prove the result is true for G with $\delta(G) = 2$.

Case 1. There exists a vertex u of degree two such that the neighbors of u have degree at least three.

Let $N(u) = \{u_1, u_2\}$ and $3 \le d(u_i) \le n-2$ for $i = 1, 2$, then $\delta(G-u) \ge 2$ and $G-u$ is triangle-free. $H(G-u) \ge h_2(n-1)$ by the induction hypothesis.

$$\begin{aligned} H(G) = & \; H(G-u) + \tfrac{2}{d(u_1)+2} + \tfrac{2}{d(u_2)+2} + \sum_{v \in N(u_1)\setminus\{u\}} \left(\tfrac{2}{d(u_1)+d(v)} - \tfrac{2}{d(u_1)+d(v)-1}\right) \\ & + \sum_{v \in N(u_2)\setminus\{u\}} \left(\tfrac{2}{d(u_2)+d(v)} - \tfrac{2}{d(u_2)+d(v)-1}\right) \\ \ge & \; H(G-u) + \tfrac{2}{d(u_1)+2} + \tfrac{2}{d(u_2)+2} + (d(u_1)-1)\left(\tfrac{2}{d(u_1)+2} - \tfrac{2}{d(u_1)+1}\right) \\ & + (d(u_2)-1)\left(\tfrac{2}{d(u_2)+2} - \tfrac{2}{d(u_2)+1}\right) \\ & \text{(with equality if and only if } d(v) = 2 \text{ for all } v \in N(u_1) \cup N(u_2) \setminus \{u\}) \\ = & \; H(G-u) + \tfrac{4}{d(u_1)+1} - \tfrac{4}{d(u_1)+2} + \tfrac{4}{d(u_2)+1} - \tfrac{4}{d(u_2)+2} \\ \ge & \; H(G-u) + \tfrac{4}{n-1} - \tfrac{4}{n} + \tfrac{4}{n-1} - \tfrac{4}{n} \\ & \text{(with equality if and only if } d(u_1) = d(u_2) = n-2) \\ \ge & \; h_2(n-1) + \tfrac{8}{n-1} - \tfrac{8}{n} \;\; \text{(with equality if and only if } G-u = K_{2,n-3}) \\ = & \; h_2(n) \end{aligned}$$

with equality if and only if $G = K_{2,n-2}$.

Case 2. Every vertex u of degree two has a neighbor of degree two in G.

Let $N(u) = \{u_1, u_2\}$ and $d(u_1) = 2$, $d(u_2) \ge 2$; $N(u_1) = \{u, v\}$.

Subcase 2.1. v is not a neighbor of u_2.

Let $G_1 = G - u + u_1u_2$, then $\delta(G_1) \ge 2$ and G_1 is triangle-free. $H(G_1) \ge h_2(n-1)$ by the induction hypothesis.

$$H(G) = H(G_1) + \frac{1}{2} \ge h_2(n-1) + \frac{1}{2} > h_2(n).$$

Subcase 2.2. v is also a neighbor of u_2.

(I) If $d(v) = d(u_2) = 2$, let $G_2 = G - u - v - u_1 - u_2$, then $\delta(G_2) \ge 2$ and G_2 is triangle-free, implying $n \ge 8$. $H(G_2) \ge h_2(n-4)$ by the induction hypothesis.

$$H(G) = H(G_2) + 2 \ge h_2(n-4) + 2 > h_2(n).$$

(II) If none of v, u_2 has degree two, then $3 \le d(v) \le n-3$ and $3 \le d(u_2) \le n-3$ since G is triangle-free. Let $G_3 = G - u - u_1$, then $\delta(G_3) \ge 2$ and G_3 is triangle-free, implying $n \ge 6$. $H(G_3) \ge h_2(n-2)$ by the induction hypothesis.

Note that $t(x,y) = \frac{2}{x+y} - \frac{2}{x+y-2} + \frac{6}{x+1} + \frac{6}{y+1} - \frac{6}{x+2} - \frac{6}{y+2} \ge t(n-3, n-3)$ for $3 \le x \le n-3$ and $3 \le y \le n-3$, since $\frac{\partial}{\partial y}(\frac{\partial t}{\partial x}) = \frac{4}{(x+y)^3} - \frac{4}{(x+y-2)^3} < 0$ and $\frac{\partial t}{\partial x} \le \frac{\partial t(x,3)}{\partial x} = -\frac{2(2x^3+21x^2+60x+49)}{(x+1)^2(x+2)^2(x+3)^2} < 0$, and $\frac{\partial t}{\partial y} < 0$, similarly.

$$\begin{aligned} H(G) = & \; H(G_3) + \tfrac{1}{2} + \tfrac{2}{d(v)+2} + \tfrac{2}{d(u_2)+2} + \tfrac{2}{d(v)+d(u_2)} - \tfrac{2}{d(v)+d(u_2)-2} \\ & + \sum_{w \in N(v)\setminus\{u_1,u_2\}} \left(\tfrac{2}{d(w)+d(v)} - \tfrac{2}{d(w)+d(v)-1}\right) \\ & + \sum_{w \in N(u_2)\setminus\{u,v\}} \left(\tfrac{2}{d(u_2)+d(w)} - \tfrac{2}{d(u_2)+d(w)-1}\right) \\ \ge & \; H(G_3) + \tfrac{1}{2} + \tfrac{2}{d(v)+2} + \tfrac{2}{d(u_2)+2} + \tfrac{2}{d(v)+d(u_2)} - \tfrac{2}{d(v)+d(u_2)-2} \\ & + (d(v)-2)\left(\tfrac{2}{d(v)+2} - \tfrac{2}{d(v)+1}\right) + (d(u_2)-2)\left(\tfrac{2}{d(u_2)+2} - \tfrac{2}{d(u_2)+1}\right) \\ = & \; H(G_3) + \tfrac{1}{2} + t(d(v), d(u_2)) \\ \ge & \; H(G_3) + \tfrac{1}{2} + t(n-3, n-3) \\ \ge & \; h_2(n-2) + \tfrac{1}{2} + t(n-3, n-3) \\ > & \; h_2(n). \end{aligned}$$

(III) If exactly one of v, u_2 has degree two, without loss of generality, assume $d(u_2) = 2$, then $3 \le d(v) \le n-3$ since G is triangle-free.

(i)If $d(v) \ge 4$, let $G_4 = G-u-u_1-u_2$, then $\delta(G_4) \ge 2$ and G_4 is triangle-free, implying $n \ge 7$. $H(G_4) \ge h_2(n-3)$ by the induction hypothesis.

$$\begin{aligned} H(G) = &\ H(G_4) + 1 + \tfrac{4}{d(v)+2} + \sum_{w\in N(v)\setminus\{u_1,u_2\}} \left(\tfrac{2}{d(w)+d(v)} - \tfrac{2}{d(w)+d(v)-2}\right) \\ \ge &\ H(G_4) + 1 + \tfrac{4}{d(v)+2} + (d(v)-2)\left(\tfrac{2}{d(v)+2} - \tfrac{2}{d(v)}\right) \\ = &\ H(G_4) + 1 + \tfrac{4}{d(v)} - \tfrac{4}{d(v)+2} \\ \ge &\ H(G_4) + 1 + \tfrac{4}{n-3} - \tfrac{4}{n-1} \\ \ge &\ h_2(n-3) + 1 + \tfrac{4}{n-3} - \tfrac{4}{n-1} \\ > &\ h_2(n) \end{aligned}$$

(ii)If $d(v) = 3$, denote by u_3 the neighbor of v in G different from u_1 and u_2.

(a) If $d(u_3) = 2$, let u_4 be the neighbor of u_3 in G different from v and $G_5 = G - u_3 + vu_4$, then $\delta(G_5) \ge 2$ and G_5 is triangle-free. $H(G_5) \ge h_2(n-1)$ by the induction hypothesis. And

$$\begin{aligned} H(G) = &\ H(G_5) + \tfrac{2}{5} + \tfrac{2}{d(u_4)+2} - \tfrac{2}{d(u_4)+3} \\ \ge &\ H(G_5) + \tfrac{2}{5} + \tfrac{2}{2+3} - \tfrac{2}{2+2} \\ = &\ H(G_5) + \tfrac{1}{2} \ge h_2(n-1) + \tfrac{1}{2} > h_2(n). \end{aligned}$$

(b) If $d(u_3) \ge 3$, then $d(u_3) \le n-5$ as G is triangle-free. Let $G_6 = G-u-v-u_1-u_2$, we have $\delta(G_6) \ge 2$ and G_6 is triangle-free, implying $n \ge 8$. $H(G_6) \ge h_2(n-4)$ by the induction hypothesis. Note that $\frac{2}{x+3} - \frac{6}{x+2} + \frac{4}{x+1}$ is decreasing for $x \ge 0$.

$$\begin{aligned} H(G) = &\ H(G_6) + 1 + \tfrac{4}{5} + \tfrac{2}{d(u_3)+3} + \sum_{w\in N(u_3)\setminus\{v\}} \left(\tfrac{2}{d(u_3)+d(w)} - \tfrac{2}{d(u_3)+d(w)-1}\right) \\ \ge &\ H(G_6) + \tfrac{9}{5} + \tfrac{2}{d(u_3)+3} + (d(u_3)-1)\left(\tfrac{2}{d(u_3)+2} - \tfrac{2}{d(u_3)+1}\right) \\ = &\ H(G_6) + \tfrac{9}{5} + \tfrac{2}{d(u_3)+3} - \tfrac{6}{d(u_3)+2} + \tfrac{4}{d(u_3)+1} \\ \ge &\ H(G_6) + \tfrac{9}{5} + \tfrac{2}{n-2} - \tfrac{6}{n-3} + \tfrac{4}{n-4} \\ \ge &\ h_2(n-4) + \tfrac{9}{5} + \tfrac{2}{n-2} - \tfrac{6}{n-3} + \tfrac{4}{n-4} \\ > &\ h_2(n). \end{aligned}$$

The proof of our theorem is completed.

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