

On Harmonic Index and Diameter of Unicyclic Graphs

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ABSTRACT. The Harmonic index $H(G)$ of a graph G is defined as the sum of the weights $\frac{2}{d(u) + d(v)}$ of all edges uv of G , where $d(u)$ denotes the degree of the vertex u in G . In this work, we prove the conjecture $\frac{H(G)}{D(G)} \geq \frac{1}{2} + \frac{1}{3(n-1)}$ given by Jianxi Liu in 2013 when G is a unicyclic graph and give a better bound $\frac{H(G)}{D(G)} \geq \frac{1}{2} + \frac{2}{3(n-2)}$, where n is the order and $D(G)$ is the diameter of the graph G .

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1. INTRODUCTION

Let $G = (V, E)$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex v of G is denoted by $d(v)$. If $u, v \in V(G)$, then the distance between u and v is the length of a shortest $u - v$ path in G . The eccentricity of a vertex v is the greatest distance from v to any other vertex of G . The diameter of a graph is the maximum over eccentricities of all vertices of the graph and it is denoted by $D(G)$. For a graph G , the harmonic index $H(G)$ is defined as $H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}$. As far as

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we know, this index first appeared in [4]. Zhong found the minimum and maximum values of the harmonic index for simple connected graphs, trees and unicyclic graphs and characterized the corresponding extremal graphs[8][9]. Wu *et al.* gave a best possible lower bound for the harmonic index of a triangle-free graph with minimum degree at least two and characterized the extremal graphs[7]. Deng *et al.* considered the relation connecting 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[3]. Mehdi Sabzevari *et al.* gave the exact formula for Merrifield Simmons and Hosoya indices of some special graphs namely ladder graph, prism graph and book graph[6]. Zohreh Bagheria *et al.* computed the edge-Szeged and vertex-PI indices of some important classes of benzenoid systems[10]. Liu proved that $H(T) - D(T) \geq \frac{5}{6} - \frac{n}{2}$ and $\frac{H(T)}{D(T)} \geq \frac{1}{2} + \frac{1}{3(n-1)}$ for n -vertex tree T with equality for path and proposed it as a conjecture for any connected graph of order n [5]. The first part of the above conjecture was proved in [1] for unicyclic graphs. In this work, we prove the second part of the conjecture viz. $\frac{H(G)}{D(G)} \geq \frac{1}{2} + \frac{2}{3(n-2)}$ for $n \geq 7$, when G is a unicyclic graph.

We conclude this section with some notations and terminology. Let $G = (V, E)$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. If $d(v) = 1$, then v is said to be a pendant vertex of G . The edge incident with v is referred to as pendant edge and the vertex adjacent to v is referred as the support vertex of v . The set of neighbours of v is denoted by $N(v)$. A diametrical path of a graph is a shortest path whose length is equal to the diameter of the graph. As usual, C_n and P_n denote the cycle and the path on n vertices, respectively. In a cycle C_n , two vertices, say u and v are said to be diametrically opposite, if $d(u, v) = \frac{n}{2}$, when n is even and $d(u, v) = \frac{n-1}{2}$, when n is odd. Let $U_{n,l}^{x,y}$ be a unicyclic graph obtained from a cycle C_l by attaching two paths P_x and P_y to two diametrically opposite vertices of C_l such that $n = l + x + y$. For other notations in graph theory, may be consulted [2].

2. BASIC RESULTS

Lemma 1. *The function $f(x) = \frac{1}{u+x} - \frac{1}{u+x-1}$ is an increasing function on x for $x \geq 1$ and $u \geq 0$.*

Lemma 2. *Let v be a pendant vertex of a connected graph G . Then $H(G) > H(G - v)$.*

Proof. Let u be the support vertex of v . Then

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

Hence $H(G) > H(G - v)$. \square

Analysing the unicyclic graphs and its diametrical path, we have the following observation.

Observation:

If $G \not\cong C_n$ is a unicyclic graph on n vertices, then at least one of the end vertices of the diametrical path of G must be a pendant vertex.

3. MAIN RESULT

In this section, we give the sharp lower bound of the relationship involving the harmonic index and diameter of connected unicyclic graphs.

Theorem 3.1. Let G be a unicyclic graph of order $n \geq 7$ and diameter $D(G)$.

Then $\frac{H(G)}{D(G)} \geq \frac{1}{2} + \frac{2}{3(n-2)}$, where equality holds if and only if $G \cong U_{n,4}^{1,n-5}$.

Proof. **Case 1:** Let $G \cong C_n$. Then $H(G) = \frac{n}{2}$. If n is even, then $D(G) = \frac{n}{2}$.

Hence $\frac{H(G)}{D(G)} = 1 \geq \frac{1}{2} + \frac{2}{3(n-2)}$. If n is odd, then $D(G) = \frac{n-1}{2}$. Hence

$$\frac{H(G)}{D(G)} = 1 + \frac{1}{n-1} \geq \frac{1}{2} + \frac{2}{3(n-2)}.$$

Case 2: Let $G \not\cong C_n$. Then G has at least one pendant vertex. Also by the observation, at least one of the end vertices of the diametrical path of G is a pendant vertex. Let P be a diametrical path of G . Now continue to remove pendant vertices from G so that P remains its diametrical path. Let the resulting graph be G' and v_1, v_2, \dots, v_k be the vertices in the order they were deleted. Then we have,

$$H(G) > H(G - v_1) > \dots > H(G - \bigcup_{i=1}^k v_i) = H(G')$$

by lemma 2 and

$$D(G) = D(G - v_1) = \dots = D(G - \bigcup_{i=1}^k v_i) = D(G').$$

Clearly G' is also a unicyclic graph consisting of a cycle of length l together with at most two pendant paths, say P_x and P_y incident with two vertices of C_l , say u and v , such that $n = k + l + x + y$.

Subcase 2.1: Let $x = 0$ and $y = 1$. In this case, $G' \cong U_{n-k, n-k-1}^{0,1}$. Then $H(G') = \frac{n-k}{2} - \frac{1}{5}$. If l is even, then $D(G') = \frac{n-k+1}{2}$. Hence

$$\begin{aligned} \frac{H(G')}{D(G')} &= \frac{5n-5k-2}{5(n-k+1)} \\ &= 1 - \frac{7}{5(n-k+1)} \\ &\geq \frac{1}{2} + \frac{2}{3(n-2)}, \quad \text{since } n-k \geq 5. \end{aligned}$$

If l is odd, then $D(G') = \frac{n-k}{2}$. Hence

$$\begin{aligned} \frac{H(G')}{D(G')} &= \frac{5n-5k-2}{5(n-k)} \\ &= 1 - \frac{2}{5(n-k)} \\ &\geq \frac{1}{2} + \frac{2}{3(n-2)}, \quad \text{since } n-k \geq 4. \end{aligned}$$

Subcase 2.2: Let $x = 0$ and $y \geq 2$. In this case, $H(G') = \frac{n-k}{2} - \frac{2}{15}$. If l is even, then $D(G') = \frac{n-k+y}{2}$. Hence

$$\begin{aligned} \frac{H(G')}{D(G')} &= \frac{15n-15k-4}{15(n-k+y)} \\ &= 1 - \frac{15y+4}{15(n-k+y)} \\ &= \frac{1}{2} + \frac{15l-8}{30(2(n-k)-l)} \\ &\geq \frac{1}{2} + \frac{2}{3(n-2)}, \quad \text{since } n-k = l+y \text{ and } l \geq 4. \end{aligned}$$

If l is odd, then $D(G') = \frac{n-k+y-1}{2}$. Hence

$$\begin{aligned} \frac{H(G')}{D(G')} &= \frac{15n-15k-4}{15(n-k+y-1)} \\ &= 1 - \frac{15y-11}{15(n-k+y-1)} \\ &= \frac{1}{2} + \frac{15l+7}{30(2(n-k)-l-1)} \\ &\geq \frac{1}{2} + \frac{2}{3(n-2)}, \quad \text{since } n-k=l+y \text{ and } l \geq 3. \end{aligned}$$

Subcase 2.3: Let $x=1, y=1$. If u and v are non adjacent, then $G' \cong U_{n-k,l}^{1,1}$.

Clearly $H(G') = \frac{n-k}{2} - \frac{2}{5}$. If l is even, then $D(G') = \frac{n-k}{2} + 1$. Hence

$$\begin{aligned} \frac{H(G')}{D(G')} &= \frac{5n-5k-4}{5(n-k+2)} \\ &= 1 - \frac{14}{5(n-k+2)} \\ &= 1 - \frac{14}{5(l+4)}, \quad \text{since } n-k=l+2 \\ &\geq \frac{1}{2} + \frac{2}{3(n-2)}. \end{aligned}$$

If l is odd, then $D(G') = \frac{n-k+1}{2}$. Hence

$$\begin{aligned} \frac{H(G')}{D(G')} &= \frac{5n-5k-4}{5(n-k+1)} \\ &= 1 - \frac{9}{5(n-k+1)} \\ &= 1 - \frac{9}{5(l+3)}, \quad \text{since } n-k=l+2 \\ &\geq \frac{1}{2} + \frac{2}{3(n-2)}. \end{aligned}$$

Subcase 2.4: Let $x=1$ and $y \geq 2$. If u and v are adjacent, the only possible graph is shown in figure 1.



FIGURE 1. G'

Clearly $H(G') = \frac{n-k}{2} - \frac{3}{10}$ and $D(G') = y + 2$. Hence

$$\begin{aligned}\frac{H(G')}{D(G')} &= \frac{5n-5k-3}{10(y+2)} \\ &\geq \frac{5n-5k-3}{10(n-2)} \\ &= 1 - \frac{5n+5k-17}{10(n-2)} \\ &\geq \frac{1}{2} + \frac{2}{3(n-2)}.\end{aligned}$$

If u and v are non adjacent, then $G' \cong U_{n-k,l}^{1,y}$. Clearly $H(G') = \frac{n-k}{2} - \frac{1}{3}$. If l is even, then $D(G') = \frac{n-k+y+1}{2}$. Hence

$$\begin{aligned}\frac{H(G')}{D(G')} &= \frac{3n-3k-2}{3(n-k+y+1)} \\ &= 1 - \frac{3y+5}{3(n-k+y+1)} \\ &\geq \frac{1}{2} + \frac{2}{3(n-2)}.\end{aligned}$$

If l is odd, then $D(G') = \frac{n-k+y}{2}$. Hence

$$\begin{aligned}\frac{H(G')}{D(G')} &= \frac{3n-3k-2}{3(n-k+y)} \\ &= 1 - \frac{3y+2}{3(n-k+y)} \\ &\geq \frac{1}{2} + \frac{2}{3(n-2)}.\end{aligned}$$

Subcase 2.5: Let $x \geq 2$ and $y \geq 2$. If u and v are adjacent, then $H(G') = \frac{n-k}{2} - \frac{7}{30}$ and $D(G') = x+y+1 = n-k-l+1$. Hence

$$\begin{aligned}\frac{H(G')}{D(G')} &= \frac{15n-15k-7}{30(n-k-l+1)} \\ &\geq \frac{1}{2} + \frac{2}{3(n-2)}.\end{aligned}$$

If u and v are non adjacent, then $H(G') = H(U_{n-k,l}^{x,y}) = \frac{n-k}{2} - \frac{4}{15}$ and $D(G') \leq D(U_{n-k,l}^{x,y})$. If l is even, $D(G') \leq \frac{n-k+x+y}{2}$. Hence

$$\begin{aligned} \frac{H(G')}{D(G')} &\geq \frac{15n-15k-8}{15(n-k+x+y)} \\ &= \frac{15n-15k-8}{15(2(n-k)-l)} \\ &= \frac{1}{2} + \frac{15l-16}{30(2(n-k)-l)} \\ &\geq \frac{1}{2} + \frac{2}{3(n-2)}. \end{aligned}$$

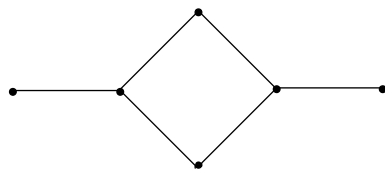
If l is odd, $D(G') \leq \frac{n-k+x+y-1}{2}$. Hence

$$\begin{aligned} \frac{H(G')}{D(G')} &\geq \frac{15n-15k-8}{15(n-k+x+y-1)} \\ &= \frac{15n-15k-8}{15(2(n-k)-l-1)} \\ &= \frac{1}{2} + \frac{15l-1}{30(2(n-k)-l-1)} \\ &\geq \frac{1}{2} + \frac{2}{3(n-2)}. \end{aligned}$$

For proving the equality, assume that $\frac{H(G)}{D(G)} = \frac{1}{2} + \frac{2}{3(n-2)}$. Since $D(G) \leq n-2$, $\frac{H(G)}{n-2} \leq \frac{H(G)}{D(G)}$, for all G . So our search is to find that G , for which $D(G) = n-2$ and $\frac{H(G)}{D(G)} = \frac{1}{2} + \frac{2}{3(n-2)}$. $U_{n,3}^{0,n-3}$, $U_{n,3}^{1,n-4}$, $U_{n,3}^{2,n-5}$, $U_{n,4}^{0,n-4}$, $U_{n,4}^{1,n-5}$ and $U_{n,4}^{2,n-6}$ are the unicyclic graphs with $D(G) = n-2$. But $U_{n,4}^{1,n-5}$ is the only graph that satisfies the equality. Hence $G \cong U_{n,4}^{1,n-5}$ and it is easy to check $\frac{H(U_{n,4}^{1,n-5})}{D(U_{n,4}^{1,n-5})} = \frac{1}{2} + \frac{2}{3(n-2)}$. □

Remark 3.1. If $n \leq 6$, this lower bound is not true. One such graph is shown in figure 2. For this graph, $\frac{H(G)}{D(G)} = \frac{13}{20} \leq \frac{2}{3} = \frac{1}{2} + \frac{2}{3(n-2)}$.

This result seems true for any connected graph of order n , that is not a tree, and we propose it as a conjecture as follows.

FIGURE 2. G

Conjecture 1. Let G be a simple connected graph, that is not a tree, of order $n \geq 7$ and diameter $D(G)$. Then $H(G) - D(G) \geq \frac{5}{3} - \frac{n}{2}$ and $\frac{H(G)}{D(G)} \geq \frac{1}{2} + \frac{2}{3(n-2)}$, where equality holds if and only if $G \cong U_{n,4}^{1,n-5}$.

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