

Note on the harmonic index of a graph

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Abstract

The harmonic index of a graph G is defined as the sum of weights $\frac{2}{deg(v)+deg(u)}$ of all edges uv of $E(G)$, where $deg(v)$ denotes the degree of a vertex v in $V(G)$. In this note we generalize results of [L. Zhong, *The harmonic index on graphs*, Appl. Math. Lett. 25 (2012), 561–566] and establish some upper and lower bounds on the harmonic index of G .

Key words: harmonic index, Randić index, trees.

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1 Introduction

Let $G = (V, E)$ be a connected simple graph with $n = |V|$ vertices and $m = |E|$ edges. The degree of a vertex v is denoted as $deg(v)$.

The Randić index is one of the most successful molecular descriptors in structure-property and structure-activity relationships studies. The Randić index $R(G)$ is defined as [8]

$$R(G) = \sum_{uv \in E} \frac{1}{\sqrt{deg(u)deg(v)}}.$$

The mathematical properties of this graph invariant have been studied extensively (see recent book [4] and survey [7]). Motivated by the success of Randić index, various generalizations and modifications were introduced, such as the sum-connectivity index [9, 11] and the general sum-connectivity index [1, 2].

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

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

In [3] the authors considered the relation between the harmonic index and the eigenvalues of graphs. Zhong in [10] presented the minimum and maximum values of harmonic index on simple connected graphs and trees, and characterized the corresponding extremal graphs. In this paper, we generalize some of these results and present alternative simpler proofs of the theorems from [10].

2 Lower bounds

Let G be a graph for which holds $deg(u) + deg(v) \leq n$ for all edges $uv \in E(G)$. In triangle-free graphs no two neighboring vertices have a common neighbor, and therefore all triangle-free graphs (trees in particular) belong to this class.

It can be easily seen that

$$H(G) \geq \sum_{uv \in E(G)} \frac{2}{n} = \frac{2m}{n}.$$

The equality holds if and only if $deg(u) + deg(v) = n$ for all edges $e = uv \in E(G)$. In particular, for triangle-free graphs the equality holds if and only if G is isomorphic to a complete bipartite graph $K_{a,b}$, $a + b = n$.

Corollary 2.1 *Let T be a tree on $n \geq 3$ vertices. Then $H(T) \geq \frac{2(n-1)}{n}$ with equality if and only if $T \cong S_n$.*

This generalizes Theorem 1 from [10].

Let $\frac{2}{deg(v) + deg(u)}$ be the weight of an edge $e = uv$. Consider an edge $e = uv$ with minimal weight among all edges of G , and let $deg(v) = p$ and $deg(u) = q$, with $p, q \geq 2$. Let x_1, x_2, \dots, x_p be the neighbors of the vertex v and y_1, y_2, \dots, y_q be the neighbors of u . Note that we allow that $x_i \equiv y_j$ for some some vertices x_i and y_j . Assume that $G' = G - e$ is a connected

graph. Then by using $p + q \geq p + \deg(x_i)$ and $p + q \geq q + \deg(y_j)$, we have

$$\begin{aligned}
 H(G) - H(G') &= \left(\frac{2}{p+q} + \sum_{i=1}^p \frac{2}{p + \deg(x_i)} + \sum_{j=1}^q \frac{2}{q + \deg(y_j)} \right) \\
 &\quad - \left(\sum_{i=1}^p \frac{2}{p-1 + \deg(x_i)} + \sum_{j=1}^q \frac{2}{q-1 + \deg(y_j)} \right) \\
 &= \frac{2}{p+q} - \sum_{i=1}^p \frac{2}{(p + \deg(x_i))(p-1 + \deg(x_i))} \\
 &\quad - \sum_{j=1}^q \frac{2}{(q + \deg(y_j))(q-1 + \deg(y_j))} \\
 &\leq \frac{2}{p+q} - \frac{2p}{(p+q)(p+q-1)} - \frac{2q}{(p+q)(p+q-1)} \\
 &= \frac{2}{p+q} - \frac{2}{p+q-1} < 0.
 \end{aligned}$$

Finally, it follows that by removing an edge with the minimal weight, the harmonic index of a graph strictly decreases.

The first Zagreb index is one of the oldest molecular structure-descriptors [5, 6] and defined as the sum of squares of the degrees of the vertices

$$M_1(G) = \sum_{v \in V} \deg(v)^2.$$

By using Cauchy-Schwarz inequality, we get

$$\left(\sum_{uv \in E(G)} \frac{2}{\deg(u) + \deg(v)} \right) \left(\sum_{uv \in E(G)} \frac{\deg(u) + \deg(v)}{2} \right) \geq \left(\sum_{e \in E(G)} 1 \right)^2,$$

or equivalently

$$H(G) \geq \frac{2m^2}{M_1(G)},$$

with equality if and only if $\deg(u) + \deg(v)$ is a constant for each edge $e = uv$ from G .

3 Upper bounds

Theorem 3.1 *Let w be a vertex of a nontrivial connected graph G . For nonnegative integers p and q , let $G(p, q)$ denote the graph obtained from G by attaching to the vertex w pendent paths $P = wv_1v_2 \dots v_p$ and $Q = wu_1u_2 \dots u_q$ of lengths p and q , respectively. Then*

$$H(G(p, q)) < H(G(p + q, 0)).$$

Proof. Without loss of generality, assume that $p \geq q > 0$. Since G is a nontrivial connected graph, we have $x = \text{deg}(w) > 2$, and after transformation the vertex degree of w decreases by one and the weights of the edges in G either remain the same or decrease (the later are the edges adjacent to w). We will consider the difference $\Delta = H(G(p + q, 0)) - H(G(p, q))$ in three cases.

Case 1. $p = q = 1$

$$\Delta > \frac{1}{x+1} + \frac{1}{3} - \frac{1}{x+1} - \frac{1}{x+1} = \frac{1}{3} - \frac{1}{x+1} > 0.$$

Case 2. $p > q = 1$

$$\Delta > \frac{1}{x+1} + \frac{1}{3} + \frac{p-1}{4} - \frac{1}{x+1} - \frac{1}{x+2} - \frac{p-2}{4} - \frac{1}{3} = \frac{1}{4} - \frac{1}{x+2} > 0.$$

Case 3. $p \geq q > 1$

$$\Delta > \frac{1}{x+1} + \frac{1}{3} + \frac{p+q-2}{4} - \frac{2}{x+2} - \frac{p+q-4}{4} - \frac{2}{3} = \frac{1}{6} - \frac{2}{x+2} + \frac{1}{x+1} > 0.$$

This completes the proof. ■

By repetitive application of this transformation on branching vertices that are on the largest distance from the center of T , we have

Corollary 3.2 *Let T be a tree on $n \geq 3$ vertices. Then $H(T) \leq \frac{4}{3} + \frac{n-3}{4}$ with equality if and only if $T \cong P_n$.*

This generalizes Theorem 2 from [10].

For $n \geq 7$, using Theorem 3.1, one can conclude that the tree with the second maximum value of harmonic index is of the form $T(a, b, c)$, composed from the branching vertex v of degree 3 with three pendent paths P_a, P_b, P_c attached to v ($a + b + c + 1 = n$). Without loss of generality, assume that $a \geq b \geq c$ and

- $b = c = 1$: $H(T(a, b, c)) = \frac{1}{5} + \frac{2}{4} + \frac{1}{3} + \frac{n-5}{4}$

- $b > c = 1$: $H(T(a, b, c)) = \frac{2}{5} + \frac{2}{3} + \frac{1}{4} + \frac{n-6}{4}$

- $b \geq c > 1$: $H(T(a, b, c)) = \frac{3}{5} + \frac{3}{3} + \frac{n-7}{4}$

By direct verification, we get that trees $T(a, b, c)$ with $a \geq b \geq c > 1$ have the second maximum value of the harmonic index among trees on n vertices.

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