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Mathematical Aspects on the Harmonic Index

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Abstract

The aim of this paper is to obtain new inequalities involving the harmonic index $H(G)$ to other well-known topological indices. Moreover, we show that the computation of the harmonic index is reduced to the computation of the primary subgraphs obtained by a general decomposition of G.

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1 Introduction

A topological index is defined as a number that represents a chemical structure in graph-theoretical terms via the molecular graph, this number is used to understand some physicochemical properties of chemical compounds. Many topological indices have been introduced and studied: the Geometric-Arithmetic (see, e.g., [9], [4], [12], [14]), sum-connectivity (see, e.g., [6], [17], [18]), 1st and 2nd Zagrev (see, e.g., [1], [2], [3], [7]) and Randić indices are a few examples of these concepts. Recall that the Randić index is, the best know index, defined as:

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

and many mathematical properties of this graph invariant have been studied since its definition, as we can see by the hundreds of papers written about it (see, e.g., [9], [10], [11], [13]), and the references therein).

Through the paper we consider graphs $G = (V(G), E(G))$ simple and connected, with $n = |V(G)|$ and $m = |E(G)|$, we will denote by d_v the degree of the vertex v in $V(G)$. The concept of harmonic index was introduced in graph theory recently, but it has shown to be useful (see, e.g., [5], [12], [15], [16] and the references therein). Given a graph G, *the harmonic index of* G is defined as the sum of $\frac{2}{d_v + d_u}$ of all edges $uv \in E(G)$. The aim of this paper is to obtain new inequalities involving the harmonic index $H(G)$ and characterize graphs extremal with respect to them. In particular, we relate $H(G)$ to other well-known topological indices and we show that the computation of the harmonic index is reduced to the computation of the primary subgraphs obtained by a general decomposition of G.

2 The harmonic index and decompositions

As usual, we say that a graph G' is a subgraph of G if $V(G') \subset V(G)$ and $E(G') \subset E(G)$. Given a graph G we say that *a family of subgraphs* $\{G_1, \ldots, G_r\}$ *is a decomposition of* G if the following conditions hold

- $G = G_1 \cup \cdots \cup G_r$ and
- any two of these subgraphs intersect themselves at most in a vertex, that is

$$G_i \cap G_j = \begin{cases} \emptyset, & \text{or;} \\ \{v\}, & \text{for some } v \in V(G). \end{cases}$$

The subgraphs are called *primary subgraphs of the decomposition.*

For a graph G the harmonic index of G is defined as follows:

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v},$$

where d_u denotes the degree of the vertex u in G.

For $v \in V(G)$ we denote by $N(v)$ the set of neighbors of v, that is,

$$N(v) = \{u \in V(G) \mid uv \in E(G)\}.$$

Given a decomposition $\{G_1, \dots, G_r\}$ of G, we fix the following notation: $\mathcal{W}$ is the set of vertices $v \in G$ belonging at least to two G_i's, given a vertex $v \in \mathcal{W}$, $G_{i_1}, \dots, G_{i_k}$ is the set of primary subgraphs containing v and d_{i_j} the number of neighbors of v in G_{i_j} (thus $d_v = d_{i_1} + \cdots + d_{i_k}$). If $v \in \mathcal{W}$, we define $W(v)$ as

$$W(v) = \sum_{u \in N_G(v) - \mathcal{W}} \frac{2}{d_u + d_v} - \sum_{j=1}^{k} \sum_{u \in N_{G_{i_j}}(v) - \mathcal{W}} \frac{2}{d_{ju} + d_{i_j v}}.$$

$\mathcal{Z}$ denotes the set of edges in G with both endpoints in $\mathcal{W}$. If $e = uv \in \mathcal{Z}$, then $e \in G_i$ for a unique i, and d_u^*, d_v^* denote the degrees of u, v in G_i, respectively. If $e = uv \in \mathcal{Z}$, we define $Z(e)$ as

$$Z(e) = \frac{2}{d_u + d_v} - \frac{2}{d_u^* + d_v^*}.$$

The following result allows to compute the precise value of $H(G)$ in terms of the harmonic indices of the primary subgraphs in any decomposition.

Theorem 2.1. *Let $\{G_1, \dots, G_r\}$ be a decomposition of the graph G. Then*

$$H(G) = \sum_{i=1}^{r} H(G_i) + \sum_{v \in \mathcal{W}} W(v) + \sum_{e \in \mathcal{Z}} Z(e).$$

Proof. First of all, note that if $u, v \notin \mathcal{W}$ and $uv \in E(G)$, then the term in $H(G)$ corresponding to uv in G is equal to its corresponding term in $\sum_{i=1}^{r} H(G_i)$.
For each $v \in \mathcal{W}$ and $u \notin \mathcal{W}$ with $uv \in E(G)$, $W(v)$ replaces in the sum $\sum_{i=1}^{r} H(G_i)$ the corresponding term to uv by its correct value as edge in G. This fact holds since the degree of u is d_u both in G and in its (unique) corresponding primary subgraph.
Finally, for each $u, v \in \mathcal{W}$ with $uv \in E(G)$, $Z(uv)$ replaces in the sum $\sum_{i=1}^{r} H(G_i)$ the corresponding term to uv by its correct value as edge in G. □

In order to estimate the difference between $H(G)$ and $\sum_{i=1}^{r} H(G_i)$, Proposition 2.1 will provide bounds for $W(v)$ and $Z(uv)$. We state first the following elemental facts.

Lemma 2.1. *Given $a \in \mathbb{Z}^+$, let g_a be the function defined as*

$$g_a(x) = \frac{2}{a + x}.$$

Then g_a strictly decreases in $[1,\infty)$ and

$$|g_a'(x)| \le \frac{2}{(a+1)^2}$$

for every $x \in [1,\infty)$.

Lemma 2.2. *Let $g : [a,b] \times [a,b] \to \mathbb{R}$ be the function defined by*

$$g(x,y) = \frac{2}{x+y}$$

with $0 < a \le b$. Then

$$\frac{1}{b} \le g(x,y) \le \frac{1}{a}$$

and $g(x,y) = g(x',y')$ if and only if $x+y = x'+y'$.

Given a decomposition $\{G_1,\dots,G_r\}$ of G and $e = uv \in \mathcal{Z}$, we say that e is *maximal* or *minimal* if $d_u = d_v$ or $d_u^* = d_v^*$, respectively.
Given a graph G, Δ and δ denote the maximum and minimum degrees of G, respectively.

Proposition 2.1. *Let $\{G_1,\dots,G_r\}$ be a decomposition of the graph G. Given $e \in \mathcal{Z}$, denote by Δ_e, δ_e the maximum and minimum degrees of the primary subgraph G_i with $e \in G_i$, respectively. Then*

1. *$-1 \le \frac{1}{\Delta} - 1 \le Z(e) \le 0$, for any $e \in \mathcal{Z}$;*
2. *$|W(v)| \le \frac{2d_v}{\delta+1}(d_v - 1)$, for every $v \in \mathcal{W}$.*

Proof. We know that $d_x \ge d_x^*$ for any $x \in V$, thus $d_u + d_v \ge d_u^* + d_v^*$ which implies

$$Z(e) = \frac{2}{d_u + d_v} - \frac{2}{d_u^* + d_v^*} \le 0$$

for $e = uv \in \mathcal{Z}$. Moreover $d_x^* \ge 1$, for $x \in V$, implies $d_u^* + d_v^* \ge 2$ so that

$$\frac{2}{d_u + d_v} - 1 \le \frac{2}{d_u + d_v} - \frac{2}{d_u^* + d_v^*} = Z(e),$$

but $\Delta \ge d_x$, then

$$\frac{1}{\Delta} - 1 \le \frac{2}{d_u + d_v} - 1$$

and clearly $-1 \le \frac{1}{\Delta} - 1$.
For the second part the Mean Value Theorem and Lemma 2.1 give

$$|g_a(d_v) - g_a(d_{i_j})| = |g_a(t)|(d_v - d_{i_j})$$

for some $t \in (d_{i_j}, d_v)$. Taking $a = d_u$ we obtain

$$|g_{d_u}(d_v) - g_{d_u}(d_{i_j})| = |g_{d_u}(t)|(d_v - d_{i_j}),$$

but $|g'_a(x)| \leq \frac{2}{(a+1)^2}$, thus

$$\left| \frac{2}{d_u + d_v} - \frac{2}{d_u + d_{i_j}} \right| \leq \frac{2}{(d_u+1)^2}(d_v - d_{i_j}) \leq \frac{2}{(d_u+1)^2}(d_v - 1)$$

finally $\delta \leq d_u$ gives

$$|W(v)| \leq \frac{2d_v}{(\delta+1)^2}(d_v - 1).$$

□

Now observe that since g_{d_u} decreases in $[d_{i_j}, \infty]$ and $d_{i_j} \leq d_v \leq d_u$, then

$$g_{d_u}(d_{i_j}) \geq g_{d_u}(d_v)$$

or equivalently

$$\frac{2}{d_u + d_{i_j}} \geq \frac{2}{d_u + d_v}$$

thus $W(v) \leq 0$, for every $v \in \mathcal{W}$. The following result is a direct consequence of this fact and Theorem 2.1.

Proposition 2.2. *Let $\{G_1, \ldots, G_r\}$ be a decomposition of the graph G. If $d_v \leq d_u$ for every $v \in \mathcal{W}$ and $u \in N_G(v) - \mathcal{W}$, then*

$$H(G) \leq \sum_{i=1}^{r} H(G_i).$$

Proof. As we said before, by Theorem 2.1 we know

$$H(G) = \sum_{i=1}^{r} H(G_i) + \sum_{v \in \mathcal{W}} W(v) + \sum_{e \in \mathcal{Z}} Z(e),$$

but $W(v), Z(e) \leq 0$ for $w \in \mathcal{W}$ and $e \in \mathcal{Z}$, hence

$$H(G) \leq \sum_{i=1}^{r} H(G_i).$$

□

Corollary 2.1. *Let $\{G_1, \ldots, G_r\}$ be a decomposition of the graph G with minimum degree δ. If $d_v = \delta$ for every $v \in \mathcal{W}$, then*

$$H(G) \leq \sum_{i=1}^{r} H(G_i).$$

3 Harmonic index versus other indices

The following theorems give relations between harmonic index and other indices. Recall that the *forgotten topological index* is defined as $F(G) = \sum_{u\in V(G)} d_u^3$ (see [8]).

Theorem 3.1. *For any graph G,*

$$m(\delta+2) - \frac{F(G)}{\Delta} \le H(G) \le \frac{F(G)}{2\delta^3}.$$

Proof. Since $(d_u - d_v)^2 + (d_u - 1)^2 + (d_v - 1)^2 \ge 0$, we have

$$(d_u^2 + d_v^2) + 1 \ge (d_u d_v) + (d_u + d_v).$$

Thus,

$$(d_u^2 + d_v^2) + 1 \ge (d_u d_v) + (d_u + d_v),$$
$$\frac{d_u^2 + d_v^2}{d_u + d_v} + \frac{1}{d_u + d_v} \ge \frac{d_u d_v}{d_u + d_v} + 1.$$

Using that

$$F(G) = \sum_{u\in V(G)} d_u^3 = \sum_{uv\in E(G)} (d_u^2 + d_v^2),$$

we get $\frac{d_u^2+d_v^2}{d_u+d_v} \le \frac{d_u^2+d_v^2}{2\Delta}$ and $\frac{d_u d_v}{d_u+d_v} \ge \frac{\delta}{2}$. We have,

$$\sum_{uv\in E(G)} \frac{d_u^2 + d_v^2}{2\Delta} + \sum_{uv\in E(G)} \frac{1}{d_u + d_v} \ge \sum_{uv\in E(G)} \frac{\delta}{2} + \sum_{uv\in E(G)} 1.$$

Therefore,

$$\frac{F(G)}{2\Delta} + H(G) \ge m(\delta+2).$$

In another hand,

$$\frac{\frac{2}{d_u+d_v}}{d_u^2 + d_v^2} = \frac{2}{(d_u + d_v)(d_u^2 + d_v^2)}.$$

Since $d_u^2 + d_v^2 \ge 2d_u d_v$,

$$\frac{\frac{2}{d_u+d_v}}{d_u^2 + d_v^2} \le \frac{1}{2\delta^3}.$$

□

For the following results, recall that *first and second Zagreb indices* are given by

$$M_1(G) = \sum_{v\in V(G)} {d_v}^2 \quad \text{and} \quad M_2(G) = \sum_{uv\in E(G)} d_u d_v.$$

Proposition 3.1. *For any graph G,*

$$F(G) + m \geq M_1(G) + M_2(G).$$

Proof. Since $(d_u - d_v)^2 + (d_u - 1)^2 + (d_v - 1)^2 \geq 0$, we have

$$\sum_{uv\in E(G)} (d_u^2 + d_v^2) + \sum_{uv\in E(G)} 1 \geq \sum_{uv\in E(G)} (d_u d_v) + \sum_{uv\in E(G)} (d_u + d_v).$$

Therefore,

$$F(G) + m \geq M_1(G) + M_2(G).$$

□

Theorem 3.2. *For any graph G the following inequality holds:*

$$\frac{\delta m^2}{M_2(G)} \leq H(G) \leq \frac{M_2(G)}{\delta^3}.$$

And the equality is attained if and only if G is regular.

Proof. First note that $\frac{d_u+d_v}{d_u d_v} \leq \frac{2}{\delta}$. Since, $\sum_{uv\in E(G)} d_u d_v = M_2(G)$, we have

$$\sum_{uv\in E(G)} (d_u + d_v) \leq \frac{2}{\delta} M_2(G)$$

and Cauchy-Schwarz inequality gives

$$\begin{aligned} m^2 &= \left(\sum_{uv\in E(G)} \frac{\sqrt{d_u + d_v}}{\sqrt{d_u + d_v}} \right)^2 \\ &\leq \left(\sum_{uv\in E(G)} \frac{1}{d_u + d_v} \right) \left(\sum_{uv\in E(G)} (d_u + d_v) \right) \\ &= \frac{M_2(G)}{\delta} \sum_{uv\in E(G)} \frac{2}{d_u + d_v} = \frac{M_2(G) H(G)}{\delta}. \end{aligned}$$

Note that,

$$\frac{\frac{2}{d_u+d_v}}{d_u d_v} = \frac{2}{(d_u + d_v)(d_u d_v)} \leq \frac{2}{2\sqrt{d_u d_v}(d_u d_v)} \leq \frac{1}{\delta^3}.$$

Thus, $\frac{2}{d_u+d_v} \leq \frac{d_u d_v}{\delta^3}$ and $H(G) \leq \frac{M_2(G)}{\delta^3}$.
Furthermore, the Cauchy-Schwarz inequality becomes an equality if and only if there is a non-zero constant μ such that, for every $uv \in E(G)$,

$$\frac{1}{\sqrt{d_u + d_v}} = \mu \sqrt{d_u + d_v}, \tag{3.1}$$

that is, $d_u + d_v = \mu^{-1}$. Thus, for any $uv, uw \in E(G)$ we get

$$\mu^{-1} = d_u + d_v = d_u + d_w,$$

which implies $d_v = d_w$. So equality 3.1 is equivalent to the following assertion: for each vertex $u \in V(G)$ every neighbor of u has the same degree. G connected implies that this holds if and only if G is regular. □

The following elementary lemma will be useful for our purposes.

Lemma 3.1. *Let $g : [a, b] \times [a, b] \to \mathbb{R}$ be the function given by*

$$g(x, y) = \frac{2\sqrt{xy}}{x + y},$$

with $0 < a \le b$. Then

$$\frac{2\sqrt{ab}}{a + b} \le g(x, y) \le 1.$$

The equality in the lower bound is attained if and only if either $x = a$ and $y = b$ or $x = b$ and $y = a$; and the equality in the upper bound is attained if and only if $x = y$.

And now recall that the *Randić index* is given by

$$R(G) = \sum_{uv \in E(G)} \frac{1}{d_u d_v}.$$

Theorem 3.3. *For any graph G the following inequalities hold:*

$$\frac{2\sqrt{\Delta\delta}}{\Delta + \delta} R(G) \le H(G) \le R(G) \quad \text{and} \quad H(G) \le \frac{n}{2}.$$

And the equality in the first inequality is attained if and only if G is regular or $(\Delta, \delta)-$biregular; the equality in the other inequalities is attained if and only if G is regular.

Proof. By previous lemma, taking $a = \delta$ and $b = \Delta$ we have

$$\frac{2\sqrt{\Delta\delta}}{\Delta + \delta} \le \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)} = \frac{\frac{2}{d_u + d_v}}{\frac{1}{\sqrt{d_u d_v}}} \le 1,$$

for any $uv \in E(G)$, hence

$$\frac{2\sqrt{\Delta\delta}}{\Delta + \delta} \frac{1}{\sqrt{d_u d_v}} \le \frac{2}{d_u + d_v} \le \frac{1}{\sqrt{d_u d_v}},$$

obtaining the first and second inequalities summing over $uv \in E(G)$.
This lemma also guaranties that the equality in the first inequality is attained if and only if for each $uv \in E(G)$ either $d_u = \delta$ and $d_v = \Delta$ or viceversa, which happens if and only if G is a regular graph or a $(\Delta, \delta)-$biregular graph.
Again the lemma asserts that equality in the second inequality is attained if and only if $d_u = d_v$ for each $uv \in E(G)$, which happens if and only if G is a regular graph.
Next, again as in the sum $\sum_{uv \in E(G)}(d_u + d_v)$ each term d_u appears exactly d_u times we get

$$\sum_{uv \in E(G)} \left(\frac{1}{d_u} + \frac{1}{d_v}\right) = \sum_{u \in V(G)} d_u \frac{1}{d_u} = n.$$

Using the fact that for every $x, y > 0$

$$\frac{2}{x+y} \leq \frac{1}{2}\left(\frac{1}{x} + \frac{1}{y}\right)$$

we obtain

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v} \leq \sum_{uv \in E(G)} \frac{1}{2}\left(\frac{1}{d_u} + \frac{1}{d_v}\right) = \frac{n}{2}.$$

Thus we have $H(G) = \frac{n}{2}$ if and only if

$$\frac{2}{d_u + d_v} = \frac{1}{2}\left(\frac{1}{d_u} + \frac{1}{d_v}\right)$$

for each $uv \in E(G)$, that is, $d_u = d_v$ for each $uv \in E(G)$. □

Theorem 3.4. *For any graph G the following inequality holds:*

$$\frac{1}{2\Delta^2} M_1(G) \leq H(G) \leq \frac{1}{2\delta^2} M_1(G).$$

And the equality in each equality is attained if and only if G is regular.

Proof. We know that

$$\frac{1}{\Delta^2} \leq \frac{4}{(d_u + d_v)^2} = \frac{\frac{2}{d_u + d_v}}{\frac{d_u + d_v}{2}} \leq \frac{1}{\delta^2}$$

for every $uv \in E(G)$. Then

$$\frac{1}{\Delta^2} \frac{d_u + d_v}{2} \leq \frac{2}{d_u + d_v} \leq \frac{1}{\delta^2} \frac{d_u + d_v}{2}$$

and since

$$\sum_{uv \in E(G)} (d_u + d_v) = \sum_{u \in V(G)} {d_u}^2 = M_1(G)$$

we obtain the inequalities by summing over $uv \in E(G)$.
The equality in the first inequality is attained if and only if $\frac{1}{2}(d_u + d_v) = \Delta$, for every $uv \in E(G)$, that is, $d_u = \Delta$ for every $u \in V(G)$. Analogously for the second inequality. □

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