MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **78** (2017) 387-404

ISSN 0340 - 6253

New Results on the Harmonic Index and Its Generalizations

José M. Rodríguez[a], **José M. Sigarreta**[b]

[a] *Departamento de Matemáticas, Universidad Carlos III de Madrid, Avenida de la Universidad 30, 28911 Leganés, Madrid, Spain*
jomaro@math.uc3m.es

[b] *Facultad de Matemáticas, Universidad Autónoma de Guerrero, Carlos E. Adame No.54 Col. Garita, 39650 Acalpulco Gro., México*
jsmathguerrero@gmail.com

(Received August 8, 2016)

Abstract

In this paper we obtain new inequalities involving the harmonic index and the (general) sum-connectivity index, and characterize graphs extremal with respect to them. In particular, we improve and generalize some known inequalities and we relate this indices to other well-known topological indices.

1 Introduction

A single number, representing a chemical structure in graph-theoretical terms via the molecular graph, is called a topological descriptor and if it in addition correlates with a molecular property it is called topological index, which is used to understand physico-chemical properties of chemical compounds. Topological indices are interesting since they capture some of the properties of a molecule in a single number. Hundreds of topological indices have been introduced and studied, starting with the seminal work by Wiener in which he used the sum of all shortest-path distances of a (molecular) graph for modeling physical properties of alkanes (see [35]).

Topological indices based on end-vertex degrees of edges have been used over 40 years. Among them, several indices are recognized to be useful tools in chemical researches. Probably, the best know such descriptor is the Randić connectivity index (R) [25]. There are more than thousand papers and a couple of books dealing with this molecular descriptor (see, e.g., [16], [19], [20], [29], [30] and the references therein). During many years, scientists were trying to improve the predictive power of the Randić index. This led to the introduction of a large number of new topological descriptors resembling the original Randić index. Two of the main successors of the Randić index are the first and second Zagreb indices, denoted by M_1 and M_2, respectively, defined as

$$M_1(G) = \sum_{uv\in E(G)} (d_u + d_v) = \sum_{u\in V(G)} d_u^2, \qquad M_2(G) = \sum_{uv\in E(G)} d_u d_v,$$

where uv denotes the edge of the graph G connecting the vertices u and v, and d_u is the degree of the vertex u. These indices have attracted growing interest, see e.g., [2], [3], [13], [21] (in particular, they are included in a number of programs used for the routine computation of topological indices). Another remarkable topological descriptor is the *harmonic* index, defined in [11] as

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

This index has attracted a great interest in the lasts years (see, e.g., [7], [12], [36], [38], [39] and [40]).

With motivation from the Randić, Zagreb and harmonic indices, the sum-connectivity index X and the *general sum-connectivity index* H_α were defined by Zhou and Trinajstić in [41] and [42], respectively, as

$$X(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}}, \qquad H_\alpha(G) = \sum_{uv\in E(G)} (d_u + d_v)^\alpha,$$

with $\alpha \in \mathbb{R}$. Note that H_1 is the first Zagreb index M_1, $2H_{-1}$ is the harmonic index H, $H_{-1/2}$ is the sum-connectivity index X, etc. Some mathematical properties of the sum-connectivity index and the general sum-connectivity index were given in [8], [9], [34], [37], [40], [43] and [44].

Throughout this paper, $G = (V, E) = (V(G), E(G))$ denotes a nontrivial ($E \neq \emptyset$) nonoriented finite simple (without multiple edges and loops) connected graph. Note that the connectivity of G is not an important restriction, since if G has connected components $G_1, \dots, G_r$, then $H_\alpha(G) = H_\alpha(G_1) + \cdots + H_\alpha(G_r)$; furthermore, every molecular graph is connected. The aim of this paper is to obtain new inequalities involving the harmonic index H and its generalizations H_α, and characterize graphs extremal with respect to them. In particular, we improve and generalize some known inequalities and we relate H and H_α to other well-known topological indices.

2 Inequalities

In order to obtain bounds for H and H_α we need the following classical result, known as Polya-Szegö inequality (see [17, p.62]).

Lemma 2.1. *If $0 < n_1 \le a_j \le N_1$ and $0 < n_2 \le b_j \le N_2$ for $1 \le j \le k$, then*

$$\Big(\sum_{j=1}^{k} a_j^2\Big)^{1/2}\Big(\sum_{j=1}^{k} b_j^2\Big)^{1/2} \le \frac{1}{2}\left(\sqrt{\frac{N_1N_2}{n_1n_2}}+\sqrt{\frac{n_1n_2}{N_1N_2}}\right)\Big(\sum_{j=1}^{k} a_jb_j\Big).$$

The following result is elementary.

Lemma 2.2. *Let g be the function $g(x,y) = \frac{2\sqrt{xy}}{x+y}$ with $0 < a \le x, y \le b$. 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 $x = y$.*

The inequality for the harmonic index $H(G) \le n/2$ is well-known. In [39, Theorem 3] appears the following lower bound for $n \ge 3$

$$\frac{2(n-1)}{n} \le H(G). \tag{2.1}$$

The corollary of the next result generalizes these inequalities for $H_\alpha(G)$.

Theorem 2.3. *Let G be a nontrivial connected graph with maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}$. Then*

$$2^{\alpha-1}\Delta^{\alpha-1}M_1(G) \le H_\alpha(G) \le 2^{\alpha-1}\delta^{\alpha-1}M_1(G), \qquad \text{if } \alpha < 1,$$
$$2^{\alpha-1}\delta^{\alpha-1}M_1(G) \le H_\alpha(G) \le 2^{\alpha-1}\Delta^{\alpha-1}M_1(G), \qquad \text{if } \alpha \ge 1,$$

and the equality holds in each inequality for some $\alpha \ne 1$ if and only if G is regular.

Proof. If $\alpha \ge 1$, then

$$H_\alpha(G) = \sum_{uv\in E(G)} (d_u+d_v)^{\alpha-1}(d_u+d_v) \le (2\Delta)^{\alpha-1}M_1(G),$$
$$H_\alpha(G) = \sum_{uv\in E(G)} (d_u+d_v)^{\alpha-1}(d_u+d_v) \ge (2\delta)^{\alpha-1}M_1(G).$$

If $\alpha < 1$, then the same argument gives

$$(2\Delta)^{\alpha-1} M_1(G) \leq \sum_{uv \in E(G)} (d_u + d_v)^{\alpha-1}(d_u + d_v) \leq (2\delta)^{\alpha-1} M_1(G).$$

If the graph is regular, then the lower and upper bounds are the same, and they are equal to $H_\alpha(G)$. If some equality holds for some $\alpha \neq 1$, then $d_u + d_v$ has the same value (2δ or 2Δ) for every $uv \in E(G)$; hence, $d_u = \delta$ (or $d_u = \Delta$) for every $u \in V(G)$ and G is regular. (If $\alpha = 1$, then each inequality is a equality for every G.) ■

Corollary 2.4. *Let G be a nontrivial connected graph with n vertices, m edges, maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}$. Then*

$$2^{\alpha+1}\Delta^{\alpha-1}\frac{m^2}{n} \leq H_\alpha(G) \leq 2^\alpha \delta^{\alpha-1}\Delta m, \qquad \text{if } \alpha < 1,$$
$$2^{\alpha+1}\delta^{\alpha-1}\frac{m^2}{n} \leq H_\alpha(G) \leq 2^\alpha \Delta^{\alpha} m, \qquad \text{if } \alpha \geq 1,$$

and the equality holds in each inequality for some $\alpha \neq 1$ if and only if G is regular.

Proof. Since $4m^2/n \leq M_1(G)$ (see [10]) and $M_1(G) \leq 2m\Delta$, Theorem 2.3 gives the inequalities.

If the graph is regular, then the lower and upper bounds are the same, and they are equal to $H_\alpha(G)$. If some equality holds for some $\alpha \neq 1$, then some equality holds in Theorem 2.3 and G is regular. ■

We have the consequence for the harmonic index $H(G) \geq 2m^2/(\Delta^2 n)$, that improves (2.1) when $m > \Delta\sqrt{n-1}$. However, our result is improved by $H(G) \geq 2m^2/M_1(G) \geq m/\Delta$ in [38, Theorem 2.5].

If we use the inequality $M_1(G) \leq 2m\Delta - \delta(\Delta n - 2m)$ (see [18, Theorem 3.2]; the equality holds for regular graphs) instead of $M_1(G) \leq 2m\Delta$, we obtain the following improved upper bounds.

Corollary 2.5. *Let G be a nontrivial connected graph with n vertices, m edges, maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}$. Then*

$$2^{\alpha+1}\Delta^{\alpha-1}\frac{m^2}{n} \leq H_\alpha(G) \leq 2^{\alpha-1}\delta^{\alpha-1}\big(2m\Delta - \delta(\Delta n - 2m)\big), \qquad \text{if } \alpha < 1,$$
$$2^{\alpha+1}\delta^{\alpha-1}\frac{m^2}{n} \leq H_\alpha(G) \leq 2^{\alpha-1}\Delta^{\alpha-1}\big(2m\Delta - \delta(\Delta n - 2m)\big), \qquad \text{if } \alpha \geq 1,$$

and the equality holds in each inequality for some $\alpha \neq 1$ if and only if G is regular. In particular, the harmonic index has the upper bound

$$H(G) \leq \frac{2m(\Delta + \delta) - \Delta\delta n}{2\delta^2}.$$

We will use the following particular case of Jensen's inequality.

Lemma 2.6. *If f is a convex function in an interval I and $x_1, \dots, x_m \in I$, then*

$$f\Big(\frac{x_1 + \cdots + x_m}{m}\Big) \le \frac{1}{m}\big(f(x_1) + \cdots + f(x_m)\big).$$

Recall that a *biregular* graph is a bipartite graph for which any vertex in one side of the given bipartition has degree Δ and any vertex in the other side of the bipartition has degree δ. If there are n_1 vertices with degree δ and n_2 vertices with degree Δ, then $m = \delta n_1 = \Delta n_2$ and we deduce $\Delta\delta n = \big(\Delta + \delta\big)m$. Note that a regular graph is biregular if and only if it is bipartite.

Next, we present several inequalities relating general harmonic indices with different parameters.

Theorem 2.7. *Let G be a nontrivial connected graph with m edges, $\alpha \in \mathbb{R}$ and $\beta > 0$. Then*

$$H_\alpha(G) \ge m^{1+1/\beta} H_{-\alpha\beta}(G)^{-1/\beta},$$

and the equality is attained for some values $\alpha \neq 0$ and β if and only if G is regular or biregular.

Proof. Since $f(x) = x^{-\beta}$ is a convex function in $\mathbb{R}_+$ for each $\beta > 0$, Lemma 2.6 gives

$$\begin{aligned}\left(\frac{m}{\sum_{uv\in E(G)}(d_u + d_v)^\alpha}\right)^\beta &\le \frac{1}{m}\sum_{uv\in E(G)}(d_u + d_v)^{-\alpha\beta},\\ \frac{m}{H_\alpha(G)} &\le \frac{1}{m^{1/\beta}}\, H_{-\alpha\beta}(G)^{1/\beta}.\end{aligned}$$

Assume that $\alpha \neq 0$. Since $f(x) = x^{-\beta}$ is a strictly convex function, the equality is attained if and only if $d_u + d_v$ is constant for every $uv \in E(G)$, and this is equivalent to the following: for each vertex $u \in V(G)$, every neighbor of u has the same degree. Since G is connected, this holds if and only if G is regular or biregular. ∎

Next, we prove nonlinear relations between $H_\alpha(G)$, $H_{\alpha+\beta}(G)$ and $H_{\alpha-\beta}(G)$ which allow to obtain a family of linear inequalities (see Corollary 2.10).

Theorem 2.8. *Let G be a nontrivial connected graph with maximum degree Δ and minimum degree δ, and $\alpha, \beta \in \mathbb{R}$. Then*

$$c_{\alpha,\beta}\sqrt{H_{\alpha+\beta}(G)H_{\alpha-\beta}(G)} \le H_\alpha(G) \le \sqrt{H_{\alpha+\beta}(G)H_{\alpha-\beta}(G)}\,,$$

with

$$c_{\alpha,\beta} := \min\left\{\frac{2(\Delta\delta)^{\beta/2}}{\Delta^\beta+\delta^\beta}, \frac{2(\Delta\delta)^{\alpha/2}}{\Delta^\alpha+\delta^\alpha}\right\} = \begin{cases} \frac{2(\Delta\delta)^{\beta/2}}{\Delta^\beta+\delta^\beta}, & \text{if } |\alpha|<|\beta|, \\ \frac{2(\Delta\delta)^{\alpha/2}}{\Delta^\alpha+\delta^\alpha}, & \text{if } |\alpha|\ge|\beta|. \end{cases}$$

The lower bound is attained for every values of α,β if G is regular. The upper bound is attained for some values of α,β with $\beta\neq 0$ if and only if G is regular or biregular.

Proof. Cauchy-Schwarz inequality gives

$$\begin{aligned}\sum_{uv\in E(G)} (d_u+d_v)^\alpha &= \sum_{uv\in E(G)} (d_u+d_v)^{(\alpha+\beta)/2+(\alpha-\beta)/2} \\ &\le \Big(\sum_{uv\in E(G)} (d_u+d_v)^{\alpha+\beta}\Big)^{1/2}\Big(\sum_{uv\in E(G)} (d_u+d_v)^{\alpha-\beta}\Big)^{1/2} \\ &= \sqrt{H_{\alpha+\beta}(G)H_{\alpha-\beta}(G)}\,.\end{aligned}$$

Since

$$\begin{aligned} &\big(2\delta\big)^{(\alpha+\beta)/2} \le \big(d_u+d_v\big)^{(\alpha+\beta)/2} \le \big(2\Delta\big)^{(\alpha+\beta)/2} && \text{if } \alpha+\beta\ge 0, \\ &\big(2\Delta\big)^{(\alpha+\beta)/2} \le \big(d_u+d_v\big)^{(\alpha+\beta)/2} \le \big(2\delta\big)^{(\alpha+\beta)/2} && \text{if } \alpha+\beta\le 0, \\ &\big(2\delta\big)^{(\alpha-\beta)/2} \le \big(d_u+d_v\big)^{(\alpha-\beta)/2} \le \big(2\Delta\big)^{(\alpha-\beta)/2} && \text{if } \alpha-\beta\ge 0, \\ &\big(2\Delta\big)^{(\alpha-\beta)/2} \le \big(d_u+d_v\big)^{(\alpha-\beta)/2} \le \big(2\delta\big)^{(\alpha-\beta)/2} && \text{if } \alpha-\beta\le 0,\end{aligned}$$

Lemma 2.1 gives, if $(\alpha+\beta)(\alpha-\beta)\ge 0$ (i.e., $|\alpha|\ge|\beta|$),

$$\begin{aligned} H_\alpha(G) = \sum_{uv\in E(G)} (d_u+d_v)^\alpha &\ge \frac{\Big(\sum_{uv\in E(G)} \big(d_u+d_v\big)^{\alpha+\beta}\Big)^{1/2}\Big(\sum_{uv\in E(G)} \big(d_u+d_v\big)^{\alpha-\beta}\Big)^{1/2}}{\frac{1}{2}\Big(\big(\frac{\Delta}{\delta}\big)^{\alpha/2}+\big(\frac{\delta}{\Delta}\big)^{\alpha/2}\Big)} \\ &= \frac{2(\Delta\delta)^{\alpha/2}}{\Delta^\alpha+\delta^\alpha}\sqrt{H_{\alpha+\beta}(G)H_{\alpha-\beta}(G)} = c_{\alpha,\beta}\sqrt{H_{\alpha+\beta}(G)H_{\alpha-\beta}(G)}\,,\end{aligned}$$

and, if $(\alpha+\beta)(\alpha-\beta)<0$ (i.e., $|\alpha|<|\beta|$), then

$$\begin{aligned} H_\alpha(G) = \sum_{uv\in E(G)} (d_u+d_v)^\alpha &\ge \frac{\Big(\sum_{uv\in E(G)} \big(d_u+d_v\big)^{\alpha+\beta}\Big)^{1/2}\Big(\sum_{uv\in E(G)} \big(d_u+d_v\big)^{\alpha-\beta}\Big)^{1/2}}{\frac{1}{2}\Big(\big(\frac{\Delta}{\delta}\big)^{\beta/2}+\big(\frac{\delta}{\Delta}\big)^{\beta/2}\Big)} \\ &= \frac{2(\Delta\delta)^{\beta/2}}{\Delta^\beta+\delta^\beta}\sqrt{H_{\alpha+\beta}(G)H_{\alpha-\beta}(G)} = c_{\alpha,\beta}\sqrt{H_{\alpha+\beta}(G)H_{\alpha-\beta}(G)}\,.\end{aligned}$$

If the graph is regular, then the lower and upper bounds are the same, and they are equal to $H_\alpha(G)$. If G is biregular, then $H_t(G)=(\Delta+\delta)^t m$ and the upper bound is attained. If the upper bound is attained for some values of α,β, then $\big(d_u+d_v\big)^{(\alpha+\beta)/2}/\big(d_u+d_v\big)^{(\alpha-\beta)/2} = \big(d_u+d_v\big)^\beta$ is constant for every $uv\in E(G)$. If $\beta\neq 0$, then d_u+d_v is constant for every $uv\in E(G)$; hence, for each vertex $u\in V(G)$, every neighbor of u has the same degree, and thus G is regular or biregular. (Note that the upper bound is $H_\alpha(G)\le H_\alpha(G)$ if $\beta=0$.) ■

Theorem 2.8 with $\beta = \alpha$ has the following consequence.

Corollary 2.9. *Let G be a nontrivial connected graph with m edges, maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}$. Then*

$$\frac{2(\Delta\delta)^{\alpha/2}}{\Delta^\alpha + \delta^\alpha} \sqrt{mH_{2\alpha}(G)} \le H_\alpha(G) \le \sqrt{mH_{2\alpha}(G)}\,.$$

The lower bound is attained for every value of α if G is regular. The upper bound is attained for some $\alpha \neq 0$ if and only if G is regular or biregular.

Theorem 2.8 and the inequality $\sqrt{ab} \le \frac{s}{2}a + \frac{1}{2s}b$ (for $a, b \ge 0$ and $s > 0$) give the following family of linear inequalities.

Corollary 2.10. *Let G be a nontrivial connected graph with maximum degree Δ and minimum degree δ, $s > 0$ and $\alpha, \beta \in \mathbb{R}$. Then*

$$H_\alpha(G) \le \frac{s}{2}\, H_{\alpha+\beta}(G) + \frac{1}{2s}\, H_{\alpha-\beta}(G),$$

The following result appears in [32, Theorem 2].

Theorem 2.11. *If $\alpha \ge 1$ is an integer and $0 \le x_1, \dots, x_k \le k-1$, then*

$$(k-1)^{1-\alpha} \sum_{j=1}^{k} x_j^\alpha \le \Big(\sum_{j=1}^{k} x_j^{1/\alpha} \Big)^\alpha .$$

Theorem 2.12. *Let G be a nontrivial connected graph with m edges, maximum degree Δ and $2\Delta \le m-1$. We have for any integer $\alpha \ge 1$*

$$H_\alpha(G) \le (m-1)^{\alpha-1} H_{\frac{1}{\alpha}}(G)^\alpha .$$

Proof. We have $d_u + d_v \le 2\Delta \le m-1$. Hence, Theorem 2.11 gives for any $uv \in E(G)$

$$(m-1)^{1-\alpha} \sum_{uv \in E(G)} (d_u + d_v)^\alpha \le \Big(\sum_{uv \in E(G)} (d_u + d_v)^{1/\alpha} \Big)^\alpha .$$

■

The following results relate $H_\alpha(G)$ with $M_1(G)$ and $M_2(G)$.

Theorem 2.13. *Let G be a nontrivial connected graph with m edges and minimum degree δ, and $0 < \alpha \le 1$. Then*

$$H_\alpha(G) \le \delta^\alpha m + \alpha \delta^{\alpha-2} M_2(G).$$

Proof. We have

$$(d_u-\delta)(d_v-\delta)\geq 0,$$

$$d_ud_v+\delta^2\geq \delta(d_u+d_v),$$

$$(\delta^{-2}d_ud_v+1)^{\alpha}\geq \delta^{-\alpha}(d_u+d_v)^{\alpha}.$$

Bernoulli inequality $(1+x)^{\alpha}\leq 1+\alpha x$ for $x\geq -1$ gives

$$\delta^{-\alpha}(d_u+d_v)^{\alpha}\leq (\delta^{-2}d_ud_v+1)^{\alpha}\leq 1+\alpha\delta^{-2}d_ud_v,$$

$$\delta^{-\alpha}H_{\alpha}(G)\leq m+\alpha\delta^{-2}M_2(G).$$

■

Theorem 2.14. *Let G be a nontrivial connected graph with m edges, and $\alpha\geq 1$. Then*

$$m+\alpha M_1(G)\leq \big(H_{\alpha}(G)^{1/\alpha}+m^{1/\alpha}\big)^{\alpha}.$$

Proof. Minkowski inequality gives

$$\Big(\sum_{uv\in E(G)}\big(d_u+d_v+1\big)^{\alpha}\Big)^{1/\alpha}\leq \Big(\sum_{uv\in E(G)}\big(d_u+d_v\big)^{\alpha}\Big)^{1/\alpha}+\Big(\sum_{uv\in E(G)}1\Big)^{1/\alpha}.$$

Bernoulli inequality $(1+x)^{\alpha}\geq 1+\alpha x$ for $x\geq -1$ gives

$$\sum_{uv\in E(G)}1+\alpha\sum_{uv\in E(G)}\big(d_u+d_v\big)\leq \big(H_{\alpha}(G)^{1/\alpha}+m^{1/\alpha}\big)^{\alpha}.$$

■

The *forgotten topological index* is defined as $F(G)=\sum_{u\in V(G)}d_u^3$ (see [14]).

Theorem 2.15. *Let G be a nontrivial connected graph with n vertices, m edges, maximum degree Δ and minimum degree δ. Then*

$$H_2(G)=F(G)+2M_2(G),$$

$$H_2(G)\geq \max\Big\{4M_2(G),\ \frac{M_1(G)^2}{2m}+2M_2(G),\ \frac{M_1(G)^2}{m}\Big\}\geq \delta M_1(G)+2M_2(G),$$

$$H_2(G)\leq \min\big\{4M_2(G)+m(n-2),\ \Delta M_1(G)+2M_2(G)\big\}.$$

Proof. Since $\sum_{uv\in E(G)}\big(f(d_u)+f(d_v)\big)=\sum_{u\in V(G)}d_uf(d_u)$, we have $\sum_{uv\in E(G)}\big(d_u^2+d_v^2\big)=\sum_{u\in V(G)}d_u^3=F(G)$. Hence,

$$H_2(G)=\sum_{uv\in E(G)}\big(d_u+d_v\big)^2=\sum_{uv\in E(G)}\big(d_u^2+d_v^2\big)+\sum_{uv\in E(G)}2d_ud_v=F(G)+2M_2(G).$$

Since $d_u^2 + d_v^2 \geq 2d_ud_v$, we obtain $F(G) \geq 2M_2(G)$. This inequality, $F(G) \geq M_1(G)^2/(2m)$ and $F(G) + 2M_2(G) \geq M_1(G)^2/m$ (see [14]) give the first lower bound. The second one follows from $M_1(G)^2/(2m) \geq 2mM_1(G)/n \geq \delta M_1(G)$.

The inequality $F(G) \leq 2M_2(G) + m(n-2)$ (see [14]) and $\sum_{u\in V(G)} d_u^3 \leq \Delta M_1(G)$ give the upper bound. ■

Recall that the *variable Zagreb index* (also called *general Randić index*) is defined in [22] as

$$Z_\alpha(G) = \sum_{uv\in E(G)} (d_ud_v)^\alpha,$$

with $\alpha \in \mathbb{R} \setminus \{0\}$. The variable Zagreb index was used in the structure-boiling point modeling of benzenoid hydrocarbons. Note that $Z_{-1/2}$ is the usual Randić index, Z_1 is the second Zagreb index M_2, Z_{-1} is the modified Zagreb index [24], etc.

We have several inequalities relating H_α with the variable Zagreb index.

Theorem 2.16. *Let G be a nontrivial connected graph with maximum degree Δ and minimum degree δ, and $\alpha, \beta \in \mathbb{R}$. Then*

$$k_{\alpha,\beta}\Big(\frac{\Delta+\delta}{\sqrt{\Delta\delta}}\Big)^\alpha \sqrt{Z_\beta(G)Z_{\alpha-\beta}(G)} \leq H_\alpha(G) \leq 2^\alpha \sqrt{Z_\beta(G)Z_{\alpha-\beta}(G)}\,, \qquad \text{if } \alpha < 0,$$
$$k_{\alpha,\beta}\, 2^\alpha \sqrt{Z_\beta(G)Z_{\alpha-\beta}(G)} \leq H_\alpha(G) \leq \Big(\frac{\Delta+\delta}{\sqrt{\Delta\delta}}\Big)^\alpha \sqrt{Z_\beta(G)Z_{\alpha-\beta}(G)}\,, \qquad \text{if } \alpha \geq 0,$$

with

$$k_{\alpha,\beta} := \begin{cases} \frac{2(\Delta\delta)^{(2\beta-\alpha)/2}}{\Delta^{2\beta-\alpha}+\delta^{2\beta-\alpha}}\,, & \text{if } \beta(\alpha-\beta) < 0, \\ \frac{2(\Delta\delta)^{\alpha/2}}{\Delta^\alpha+\delta^\alpha}\,, & \text{if } \beta(\alpha-\beta) \geq 0. \end{cases}$$

Each one of the three first inequalities is attained for some values of α, β with $\alpha \neq 0$ if and only if G is regular. The last inequality is attained for some values of α, β with $\alpha \neq 0$ if and only if G is regular or biregular.

Proof. By Lemma 2.2, we have

$$2\sqrt{d_ud_v} \leq d_u + d_v \leq \frac{\Delta+\delta}{\sqrt{\Delta\delta}}\sqrt{d_ud_v}\,.$$

If $\alpha \geq 0$, then

$$2^\alpha\big(d_ud_v\big)^{\alpha/2} \leq \big(d_u+d_v\big)^\alpha \leq \Big(\frac{\Delta+\delta}{\sqrt{\Delta\delta}}\Big)^\alpha \big(d_ud_v\big)^{\alpha/2}.$$

If $\alpha < 0$, then

$$\Big(\frac{\Delta+\delta}{\sqrt{\Delta\delta}}\Big)^\alpha \big(d_ud_v\big)^{\alpha/2} \leq \big(d_u+d_v\big)^\alpha \leq 2^\alpha\big(d_ud_v\big)^{\alpha/2}.$$

Cauchy-Schwarz inequality gives

$$\sum_{uv\in E(G)} \big(d_u d_v\big)^{\alpha/2} = \sum_{uv\in E(G)} \big(d_u d_v\big)^{\beta/2+(\alpha-\beta)/2}$$

$$\le \Big(\sum_{uv\in E(G)} \big(d_u d_v\big)^{\beta}\Big)^{1/2}\Big(\sum_{uv\in E(G)} \big(d_u d_v\big)^{\alpha-\beta}\Big)^{1/2} = \sqrt{Z_\beta(G) Z_{\alpha-\beta}(G)}\,.$$

Since

$$\begin{aligned}
\delta^\beta \le \big(d_u d_v\big)^{\beta/2} &\le \Delta^\beta && \text{if } \beta > 0,\\
\Delta^\beta \le \big(d_u d_v\big)^{\beta/2} &\le \delta^\beta && \text{if } \beta < 0,\\
\delta^{\alpha-\beta} \le \big(d_u d_v\big)^{(\alpha-\beta)/2} &\le \Delta^{\alpha-\beta} && \text{if } \alpha-\beta \ge 0,\\
\Delta^{\alpha-\beta} \le \big(d_u d_v\big)^{(\alpha-\beta)/2} &\le \delta^{\alpha-\beta} && \text{if } \alpha-\beta < 0,
\end{aligned}$$

Lemma 2.1 gives, if $\beta(\alpha-\beta)\ge 0$,

$$\begin{aligned}
\sum_{uv\in E(G)} \big(d_u d_v\big)^{\alpha/2} &\ge \frac{\Big(\sum_{uv\in E(G)} \big(d_u d_v\big)^{\beta}\Big)^{1/2}\Big(\sum_{uv\in E(G)} \big(d_u d_v\big)^{\alpha-\beta}\Big)^{1/2}}{\frac{1}{2}\Big(\big(\frac{\Delta}{\delta}\big)^{\alpha/2}+\big(\frac{\delta}{\Delta}\big)^{\alpha/2}\Big)}\\
&= \frac{2(\Delta\delta)^{\alpha/2}}{\Delta^\alpha+\delta^\alpha}\sqrt{Z_\beta(G) Z_{\alpha-\beta}(G)} = k_{\alpha,\beta}\sqrt{Z_\beta(G) Z_{\alpha-\beta}(G)}\,,
\end{aligned}$$

and, if $\beta(\alpha-\beta)<0$, then

$$\begin{aligned}
\sum_{uv\in E(G)} \big(d_u d_v\big)^{\alpha/2} &\ge \frac{\Big(\sum_{uv\in E(G)} \big(d_u d_v\big)^{\beta}\Big)^{1/2}\Big(\sum_{uv\in E(G)} \big(d_u d_v\big)^{\alpha-\beta}\Big)^{1/2}}{\frac{1}{2}\Big(\big(\frac{\Delta}{\delta}\big)^{(2\beta-\alpha)/2}+\big(\frac{\delta}{\Delta}\big)^{(2\beta-\alpha)/2}\Big)}\\
&= \frac{2(\Delta\delta)^{(2\beta-\alpha)/2}}{\Delta^{2\beta-\alpha}+\delta^{2\beta-\alpha}}\sqrt{Z_\beta(G) Z_{\alpha-\beta}(G)} = k_{\alpha,\beta}\sqrt{Z_\beta(G) Z_{\alpha-\beta}(G)}\,.
\end{aligned}$$

If the graph is regular, then the lower and upper bounds are the same, and they are equal to $H_\alpha(G)$.

If the second or the third inequality is attained for some values of α,β with $\alpha\neq 0$, then $2\sqrt{d_u d_v} = d_u + d_v$ for every $uv\in E(G)$, and Lemma 2.2 gives $d_u = d_v$ for every $uv\in E(G)$; since G is connected, G is regular.

Assume now that the first or the last inequality is attained for some values of α,β with $\alpha\neq 0$. Thus, $d_u + d_v = \frac{\Delta+\delta}{\sqrt{\Delta\delta}}\sqrt{d_u d_v}$ for every $uv\in E(G)$. By Lemma 2.2, this holds if and only if every edge joins a vertex of degree δ with a vertex of degree Δ, and this is equivalent to the following: for each vertex $u\in V(G)$, we have $\deg(u)\in\{\delta,\Delta\}$, if $\deg(u)=\delta$ then every neighbor of u has degree Δ, and if $\deg(u)=\Delta$ then every neighbor of u has degree δ. Since G is connected, this holds if and only if G is regular or biregular.

If G is regular or biregular, then $\sqrt{Z_\beta(G)Z_{\alpha-\beta}(G)} = \sqrt{(\Delta\delta)^\beta m(\Delta\delta)^{\alpha-\beta}m} = (\Delta\delta)^{\alpha/2}m$ and $H_\alpha(G) = (\Delta+\delta)^\alpha m$. Hence, the last inequality is attained. If $\alpha \neq 0$, then the first inequality is attained if and only if $k_{\alpha,\beta} = 1$, and this holds if and only $\Delta = \delta$ by Lemma 2.2, i.e., G is regular. ■

We have the following consequence.

Corollary 2.17. *Let G be a nontrivial connected graph with maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}$. Then*

$$\begin{aligned} \frac{2(\Delta+\delta)^\alpha}{\Delta^\alpha+\delta^\alpha}\, Z_{\alpha/2}(G) \le H_\alpha(G) \le 2^\alpha Z_{\alpha/2}(G), \qquad & \textit{if } \alpha < 0, \\ \frac{2^{\alpha+1}(\Delta\delta)^{\alpha/2}}{\Delta^\alpha+\delta^\alpha}\, Z_{\alpha/2}(G) \le H_\alpha(G) \le \Big(\frac{\Delta+\delta}{\sqrt{\Delta\delta}}\Big)^\alpha Z_{\alpha/2}(G), \qquad & \textit{if } \alpha \ge 0. \end{aligned}$$

Each one of the three first inequalities is attained for some value of $\alpha \neq 0$ if and only if G is regular. The last inequality is attained for some value of $\alpha \neq 0$ if and only if G is regular or biregular.

In [31, Lemma 3] appears the following result.

Lemma 2.18. *Let h be the function $h(x,y) = \frac{2xy}{x+y}$ with $\delta \le x, y \le \Delta$. Then $\delta \le h(x,y) \le \Delta$. Furthermore, the lower (respectively, upper) bound is attained if and only if $x = y = \delta$ (respectively, $x = y = \Delta$).*

Theorem 2.19. *Let G be a nontrivial connected graph with m edges, maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}$. Then*

$$\begin{aligned} \frac{2^\alpha m^2}{\delta^\alpha Z_{-\alpha}(G)} \le H_\alpha(G) \le \frac{\Delta^{3\alpha/2}+\delta^{3\alpha/2}}{\Delta^{7\alpha/4}\delta^{3\alpha/4}}\,\frac{2^{\alpha-1}m^2}{Z_{-\alpha}(G)}, \qquad & \textit{if } \alpha < 0, \\ \frac{2^\alpha m^2}{\Delta^\alpha Z_{-\alpha}(G)} \le H_\alpha(G) \le \frac{\Delta^{3\alpha/2}+\delta^{3\alpha/2}}{\Delta^{3\alpha/4}\delta^{7\alpha/4}}\,\frac{2^{\alpha-1}m^2}{Z_{-\alpha}(G)}, \qquad & \textit{if } \alpha \ge 0, \end{aligned}$$

and each inequality is attained for some value of $\alpha \neq 0$ if and only if G is regular.

Proof. By Lemma 2.18, we have

$$\begin{aligned} \Big(\frac{2}{\Delta}\Big)^{\alpha/2} \le \frac{\big(d_u+d_v\big)^{\alpha/2}}{\big(d_ud_v\big)^{\alpha/2}} \le \Big(\frac{2}{\delta}\Big)^{\alpha/2}, \qquad & \text{if } \alpha \ge 0, \\ \Big(\frac{2}{\delta}\Big)^{\alpha/2} \le \frac{\big(d_u+d_v\big)^{\alpha/2}}{\big(d_ud_v\big)^{\alpha/2}} \le \Big(\frac{2}{\Delta}\Big)^{\alpha/2}, \qquad & \text{if } \alpha < 0. \end{aligned}$$

Cauchy-Schwarz inequality gives

$$\left(\sum_{uv \in E(G)} \frac{\big(d_u + d_v\big)^{\alpha/2}}{\big(d_u d_v\big)^{\alpha/2}} \right)^2 \le \Big(\sum_{uv \in E(G)} \big(d_u + d_v\big)^{\alpha} \Big) \Big(\sum_{uv \in E(G)} \big(d_u d_v\big)^{-\alpha} \Big) = H_\alpha(G) Z_{-\alpha}(G).$$

These inequalities provide the lower bounds.

Since

$$\begin{aligned} &(2\delta)^{\alpha/2} \le \big(d_u + d_v\big)^{\alpha/2} \le (2\Delta)^{\alpha/2}, \qquad \Delta^{-\alpha} \le \big(d_u d_v\big)^{-\alpha/2} \le \delta^{-\alpha}, \qquad \text{if } \alpha \ge 0, \\ &(2\Delta)^{\alpha/2} \le \big(d_u + d_v\big)^{\alpha/2} \le (2\delta)^{\alpha/2}, \qquad \delta^{-\alpha} \le \big(d_u d_v\big)^{-\alpha/2} \le \Delta^{-\alpha}, \qquad \text{if } \alpha < 0, \end{aligned}$$

Lemma 2.1 gives in both cases

$$\begin{aligned} \left(\sum_{uv \in E(G)} \frac{\big(d_u + d_v\big)^{\alpha/2}}{\big(d_u d_v\big)^{\alpha/2}} \right)^2 &\ge \frac{\Big(\sum_{uv \in E(G)} \big(d_u + d_v\big)^{\alpha} \Big) \Big(\sum_{uv \in E(G)} \big(d_u d_v\big)^{-\alpha} \Big)}{\frac{1}{2}\Big(\big(\frac{\Delta}{\delta}\big)^{3\alpha/4} + \big(\frac{\delta}{\Delta}\big)^{3\alpha/4} \Big)} \\ &= \frac{2(\Delta\delta)^{3\alpha/4}}{\Delta^{3\alpha/2} + \delta^{3\alpha/2}} H_\alpha(G) Z_{-\alpha}(G), \end{aligned}$$

and this gives the upper bounds.

If the graph is regular, then the lower and upper bounds are the same, and they are equal to $H_\alpha(G)$. If some bound is attained for some value of $\alpha \neq 0$, then Lemma 2.18 gives $d_u = d_v = \delta$ for every $uv \in E(G)$ or $d_u = d_v = \Delta$ for every $uv \in E(G)$; hence, G is regular. ■

Theorem 2.20. *Let G be a nontrivial connected graph with n vertices, and $\alpha > 1$. Then*

$$n^\alpha \le H_\alpha(G) Z_{\frac{-\alpha}{\alpha-1}}(G)^{\alpha-1},$$

and the equality is attained for some value of $\alpha > 1$ if and only if G is regular or biregular.

Proof. Recall that $\sum_{uv \in E(G)} \big(f(d_u) + f(d_v)\big) = \sum_{u \in V(G)} d_u f(d_u)$. Hence,

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

Since $\alpha > 1$, Hölder inequality gives

$$n \le \Big(\sum_{uv \in E(G)} \big(d_u + d_v\big)^{\alpha} \Big)^{\frac{1}{\alpha}} \Big(\sum_{uv \in E(G)} \big(d_u d_v\big)^{\frac{-\alpha}{\alpha-1}} \Big)^{\frac{\alpha-1}{\alpha}} = H_\alpha(G)^{\frac{1}{\alpha}} Z_{\frac{-\alpha}{\alpha-1}}(G)^{\frac{\alpha-1}{\alpha}}.$$

If G is regular or biregular, then $\Delta\delta n = \big(\Delta + \delta\big)m$, $H_\alpha(G) = (\Delta + \delta)^\alpha m$, $Z_{\frac{-\alpha}{\alpha-1}}(G) = (\Delta\delta)^{\frac{-\alpha}{\alpha-1}} m$, and the equality is attained.

If the equality is attained for some value of $\alpha > 1$, then $\big(d_u d_v\big)^{\frac{-\alpha}{\alpha-1}} / \big(d_u + d_v\big)^{\alpha}$ is constant for every $uv \in E(G)$, i.e., $d_u d_v \big(d_u + d_v\big)^{\alpha-1}$ is constant for every $uv \in E(G)$. Since the function $F(t) = d_u t \big(d_u + t\big)^{\alpha-1}$ is increasing when $t \in [1, \infty)$, we have the following: for each vertex $u \in V(G)$, every neighbor v of u has the same degree, and the degree of every neighbor of v is d_u. Since G is connected, G is regular or biregular. ∎

We have the following consequence, that improves the lower bound in Theorem 2.19 when $\alpha = 2$, since $2m \le \Delta n$.

Corollary 2.21. *Let G be a nontrivial connected graph with n vertices. Then*

$$n^2 \le H_2(G) Z_{-2}(G),$$

and the equality is attained if and only if G is regular or biregular.

The *modified Narumi-Katayama index*

$$NK^*(G) = \prod_{u \in V(G)} d_u^{d_u} = \prod_{uv \in E(G)} d_u d_v$$

is introduced in [15], inspired in the Narumi-Katayama index defined in [23]. Next, we prove several inequalities relating the modified Narumi-Katayama index with H_α.

Theorem 2.22. *Let G be a nontrivial connected graph with m edges, maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}$. Then*

$$\begin{aligned} H_\alpha(G) &\ge \Big(\frac{\Delta + \delta}{\sqrt{\Delta\delta}}\Big)^{\alpha} m \, NK^*(G)^{\alpha/(2m)}, \qquad && \text{if } \alpha < 0, \\ H_\alpha(G) &\ge 2^{\alpha} m \, NK^*(G)^{\alpha/(2m)}, \qquad && \text{if } \alpha \ge 0. \end{aligned}$$

The equality holds for some $\alpha < 0$ if and only if G is regular or biregular. The equality holds for some $\alpha > 0$ if and only if G is regular.

Proof. Using the fact that the geometric mean is at most the arithmetic mean, Lemma 2.2 gives for $\alpha \ge 0$

$$\begin{aligned} \frac{1}{m} H_\alpha(G) &= \frac{1}{m} \sum_{uv \in E(G)} (d_u + d_v)^{\alpha} \ge \frac{1}{m} \sum_{uv \in E(G)} \big(2\sqrt{d_u d_v}\,\big)^{\alpha} \\ &\ge 2^{\alpha} \Big(\prod_{uv \in E(G)} (d_u d_v)^{\alpha/2} \Big)^{1/m} = 2^{\alpha} NK^*(G)^{\alpha/(2m)}. \end{aligned}$$

Lemma 2.2 gives for $\alpha < 0$

$$\frac{1}{m} H_\alpha(G) = \frac{1}{m} \sum_{uv \in E(G)} (d_u + d_v)^\alpha \ge \frac{1}{m} \sum_{uv \in E(G)} \Big(\frac{\Delta + \delta}{\sqrt{\Delta\delta}} \sqrt{d_u d_v} \Big)^\alpha$$
$$\ge \Big(\frac{\Delta + \delta}{\sqrt{\Delta\delta}} \Big)^\alpha \Big(\prod_{uv \in E(G)} (d_u d_v)^{\alpha/2} \Big)^{1/m} = \Big(\frac{\Delta + \delta}{\sqrt{\Delta\delta}} \Big)^\alpha NK^*(G)^{\alpha/(2m)}.$$

If the graph is regular, then $H_\alpha(G) = 2^\alpha \delta^\alpha m$, $NK^*(G) = \delta^{2m}$ and we have the equality. If the graph is biregular and $\alpha < 0$, then $H_\alpha(G) = (\Delta + \delta)^\alpha m$, $NK^*(G) = (\Delta\delta)^m$ and we have the equality. If the equality holds for some $\alpha > 0$, then Lemma 2.2 gives $d_u = d_v$ for every $uv \in E(G)$; since G is a connected graph, G is regular. If the equality holds for some $\alpha < 0$, then Lemma 2.2 gives $d_u = \delta$ and $d_v = \Delta$ or vice versa for every $uv \in E(G)$; hence, G is regular or biregular. ■

The first geometric-arithmetic index GA_1 was introduced in [33] as

$$GA_1(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)} .$$

Although GA_1 was introduced in 2009, there are many papers dealing with this index (see, e.g., [4], [5], [6], [26], [27], [28], [33] and the references therein).

Theorem 2.23. *Let G be a nontrivial connected graph with m edges, maximum degree Δ and minimum degree δ. Then*

$$H(G) + \frac{1}{\sqrt{\Delta\delta}} GA_1(G) \le \frac{2m}{\delta} ,$$

and the equality holds if and only if G is regular.

Proof. Note that $\big(\sqrt{d_u} - \sqrt{\delta}\,\big)\big(\sqrt{\Delta} - \sqrt{d_v}\,\big) \ge 0$. Therefore,

$$\sqrt{\Delta}\,\big(\sqrt{d_u} + \sqrt{d_v}\,\big) \ge \sqrt{\Delta}\,\sqrt{d_u} + \sqrt{\delta}\,\sqrt{d_v} \ge \sqrt{d_u d_v} + \sqrt{\Delta\delta}\,.$$

Since $\sqrt{d_w} \le d_w/\sqrt{\delta}$ for every vertex $w \in V(G)$, we obtain

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

$$\frac{1}{\sqrt{\Delta\delta}} \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} + \sum_{uv \in E(G)} \frac{2}{d_u + d_v} \le \frac{2m}{\delta} , \qquad H(G) + \frac{1}{\sqrt{\Delta\delta}} GA_1(G) \le \frac{2m}{\delta} .$$

If the graph is regular, then $GA_1(G) = m$ and $H(G) = m/\delta$, and the equality holds. If the equality is attained, then $\sqrt{\Delta} = \sqrt{\delta}$ and G is regular. ■

Acknowledgement: The authors are grateful to the referees for their valuable comments which have improved this paper. This work is supported in part by two grants from Ministerio de Economía y Competititvidad (MTM2013-46374-P and MTM2015-69323-REDT), Spain, and a grant from CONACYT (FOMIX-CONACyT-UAGro 249818), México.

References

[1] V. Andova, M. Petruševski, Variable Zagreb indices and Karamata's inequality, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 685–690.

[2] B. Borovićanin, B. Furtula, On extremal Zagreb indices of trees with given domination number, *Appl. Math. Comput.* **279** (2016) 208–218.

[3] K. C. Das, On comparing Zagreb indices of graphs, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 433–440.

[4] K. C. Das, On geometric–arithmetic index of graphs, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 619–630.

[5] K. C. Das, I. Gutman, B. Furtula, Survey on geometric–arithmetic indices of graphs, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 595–644.

[6] K. C. Das, I. Gutman, B. Furtula, On first geometric–arithmetic index of graphs, *Discr. Appl. Math.* **159** (2011) 2030–2037.

[7] H. Deng, S. Balachandran, S. K. Ayyaswamy, Y. B. Venkatakrishnan, On the harmonic index and the chromatic number of a graph, *Discr. Appl. Math.* **161** (2013) 2740–2744.

[8] Z. Du, B. Zhou, N. Trinajstić, Minimum sum–connectivity indices of trees and unicyclic graphs of a given matching number, *J. Math. Chem.* **47** (2010) 842–855.

[9] Z. Du, B. Zhou, N. Trinajstić, On the general sum–connectivity index of trees, *Appl. Math. Lett.* **24** (2011) 402–405.

[10] C. S. Edwards, The largest vertex degree sum for a triangle in a graph, *Bull. London Math. Soc.* **9** (1977) 203–208.

[11] S. Fajtlowicz, On conjectures of Graffiti–II, *Congr. Num.* **60** (1987) 187–197.

[12] O. Favaron, M. Mahéo, J. F. Saclé, Some eigenvalue properties in graphs (conjectures of Graffiti–II), *Discr. Math.* **111** (1993) 197–220.

[13] B. Furtula, I. Gutman, S. Ediz, On difference of Zagreb indices, *Discr. Appl. Math.* **178** (2014) 83–88.

[14] B. Furtula, I. Gutman, A forgotten topological index, *J. Math. Chem.* **53** (2015) 1184–1190.

[15] M. Ghorbani, M. Songhori, I. Gutman, Modified Narumi–Katayama index, *Kragujevac J. Sci.* **34** (2012) 57–64.

[16] I. Gutman, B. Furtula (Eds.), *Recent Results in the Theory of Randić Index*, Univ. Kragujevac, Kragujevac, 2008.

[17] G. H. Hardy, J. E. Littlewood, G. Polya, *Inequalities*, Cambridge Univ. Press, Cambridge, 1952.

[18] A. Ilić, M. Ilić, B. Liu, On the upper bounds for the first Zagreb index, *Kragujevac J. Math.* **35** (2011) 173–182.

[19] X. Li, I. Gutman, *Mathematical Aspects of Randić Type Molecular Structure Descriptors*, Univ. Kragujevac, Kragujevac, 2006.

[20] X. Li, Y. Shi, A survey on the Randić index, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 127–156.

[21] M. Liu, A simple approach to order the first Zagreb indices of connected graphs, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 425–432.

[22] A. Miličević, S. Nikolić, On variable Zagreb indices, *Croat. Chem. Acta* **77** (2004) 97–101.

[23] H. Narumi, M. Katayama, Simple topological index. A newly devised index characterizing the topological nature of structural isomers of saturated hydrocarbons, *Mem. Fac. Engin. Hokkaido Univ.* **16** (1984) 209–214.

[24] S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, The Zagreb Indices 30 years after, *Croat. Chem. Acta* **76** (2003) 113–124.

[25] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.

[26] J. M. Rodríguez, J. M. Sigarreta, On the geometric–arithmetic index, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 103–120.

[27] J. M. Rodríguez, J. M. Sigarreta, Spectral study of the geometric–arithmetic index, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 121–135.

[28] J. M. Rodríguez, J. M. Sigarreta, Spectral properties of geometric–arithmetic index, *Appl. Math. Comput.* **277** (2016) 142–153.

[29] J. A. Rodríguez–Velázquez, J. M. Sigarreta, On the Randić index and conditional parameters of a graph, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 403–416.

[30] J. A. Rodríguez–Velázquez, J. Tomás–Andreu, On the Randić index of polymeric networks modelled by generalized Sierpinski graphs, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 145–160.

[31] J. M. Sigarreta, Bounds for the geometric–arithmetic index of a graph, *Miskolc Math. Notes* **16** (2015) 1199–1212.

[32] L. A. Székely, L. H. Clark, R. C. Entringer, An inequality for degree sequences, *Discr. Math.* **103** (1992) 293–300.

[33] D. Vukičević, B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end–vertex degrees of edges, *J. Math. Chem.* **46** (2009) 1369–1376.

[34] S. Wang, B. Zhou, N. Trinajstić, On the sum–connectivity index, *Filomat* **25** (2011) 29–42.

[35] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.

[36] R. Wua, Z. Tanga, H. Deng, A lower bound for the harmonic index of a graph with minimum degree at least two, *Filomat* **27** (2013) 51–55.

[37] R. Xing, B. Zhou, N. Trinajstić, Sum–connectivity index of molecular trees, *J. Math. Chem.* **48** (2010) 583–591.

[38] X. Xu, Relationships between harmonic index and other topological indices, *Appl. Math. Sci.* **6** (2012) 2013–2018.

[39] L. Zhong, The harmonic index for graphs, *Appl. Math. Lett.* **25** (2012) 561–566.

[40] L. Zhong, K. Xu, Inequalities between vertex–degree–based topological indices, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 627–642.

[41] B. Zhou, N. Trinajstić, On a novel connectivity index, *J. Math. Chem.* **46** (2009) 1252–1270.

[42] B. Zhou, N. Trinajstić, On general sum–connectivity index, *J. Math. Chem.* **47** (2010) 210–218.

[43] B. Zhou, N. Trinajstić, Relations between the product– and sum–connectivity indices, *Croat. Chem. Acta* **85** (2012) 363–365.

[44] Z. Zhu, H. Lu, On the general sum–connectivity index of tricyclic graphs, *J. Appl. Math. Comput.* **51** (2016) 177–188.