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ESTIMATING THE ZAGREB AND THE GENERAL RANDIĆ INDICES

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Abstract

The Zagreb indices were introduced 30 years ago. Since then also various modified Zagreb indices were put forward, and these all happen to be special cases of the general Randić index. In this paper we report several novel estimates of the general Randić index and of its special cases – the ordinary and modified Zagreb indices.

1. INTRODUCTION

Two molecular structure–descriptors, denoted by M_1 and M_2, were put forward 30 years ago, and are nowadays referred to as the first and second Zagreb indices.

These are defined as

$$M_1 = M_1(G) = \sum_{i=1}^{n} d_i^2 \qquad ; \qquad M_2 = M_2(G) = \sum_{i\sim j} d_i\, d_j$$

where d_i stands for the degree of the vertex i in the respective (molecular) graph G, the summation in M_1 runs over all vertices i of G whereas the summation in M_2 runs over all edges of G. The symbol $i \sim j$ indicates that the vertices i and j are adjacent.

The quantities M_1 and M_2 were first encountered within a study of the structure–dependence of the total π-electron energy [1]. Soon thereafter it was recognized that both M_1 and M_2 can be viewed as measures of molecular branching [2]. The name *Zagreb index* seems to be first used in the review [3]; M_1 and M_2 are referred to as the first and second Zagreb index, respectively [3, 4].

The Zagreb indices do not belong among the popular and frequently used structure–descriptors, but some of their applications in QSPR and QSAR studies were nevertheless attempted. For more data on this matter see the reviews [5, 6], the recent works [7–11] and the papers quoted therein. Mathematical properties of the Zagreb indices have also been much studied in the recent past [6,12–18].

In addition to the original Zagreb indices, several modified versions thereof were also introduced [5,19–22]; for details see below.

The connectivity index, also called vertex–connectivity index or Randić index, denoted by ${}^1R$, is given by

$${}^1R = {}^1R(G) = \sum_{i\sim j} \frac{1}{\sqrt{d_i\, d_j}} \ .$$

This index is also referred to as the first-order (vertex-)connectivity index. Its zeroth-order variant is defined as

$${}^0R = {}^0R(G) = \sum_{i=1}^{n} \frac{1}{\sqrt{d_i}} \ .$$

The general Randić index and the general zeroth–order Randić index are defined as

$$R_\alpha = R_\alpha(G) = \sum_{i\sim j} (d_i\, d_j)^\alpha$$

and

$$Q_\alpha = Q_\alpha(G) = \sum_{i=1}^{n} (d_i)^\alpha \ .$$

Evidently, for $\alpha = -1/2$ the general Randić index and the general zeroth–order Randić index reduce to the ordinary Randić index and the ordinary zeroth–order Randić index, respectively, i. e.,

$$^{1}R(G) = R_{-1/2}(G) \qquad ; \qquad {}^{0}R(G) = Q_{-1/2}(G) \; .$$

What also needs to be noticed is that for the general Randić index for $\alpha = 1$ and the general zeroth–order Randić index for $\alpha = 2$ reduce to the second and first Zagreb indices, respectively, i. e.,

$$M_1(G) = Q_2(G) \qquad ; \qquad M_2(G) = R_1(G) \; .$$

The theory of the Randić–type structure–descriptors is outlined in detail in the recent book [23], where the interested reader may also find an exhaustive bibliography on this matter.

The modified Zagreb indices are defined as follows

$$^{m}A = \sum_{i=1}^{n} \frac{1}{d_i} \quad ; \quad {}^{m}M_1 = \sum_{i=1}^{n} \frac{1}{d_i^2} \quad ; \quad {}^{m}M_2 = \sum_{i\sim j} \frac{1}{d_i\, d_j} \; .$$

Thus

$$^{m}A = Q_{-1}(G) \quad ; \quad {}^{m}M_1 = Q_{-2}(G) \quad ; \quad {}^{m}M_2 = R_{-1}(G)$$

and

$$^{m}M_1 \leq {}^{m}A \leq {}^{0}R \leq M_1 \quad ; \quad {}^{m}M_2 \leq {}^{1}R \leq M_2 \; .$$

In addition, $M_1(G) = M_2(G)$ if and only if G is a 2-regular graph [17]; if G is connected, then $M_1(G) = M_2(G)$ holds only if $G \cong C_n$.

In this paper we will compare above specified topological indices and estimate them.

2. COMPARING VARIOUS ZAGREB INDICES

Let $G = G(V, E)$ be a simple graph of order n and with m edges, i. e., $|V| = n$, $|E| = m$. The adjacency matrix of G is denoted by A, with $(A)_{i,j}$ being its (i, j)-th entry.

In [5], the following formula for M_1 was given, viz.,

$$M_1 = \frac{1}{2}\left[\sum_{i=1}^{n}(A^4)_{ii} + 2m\right] \,. \tag{1}$$

We would like to point out that formula (1) is correct only for graphs that are C_4-free. In fact, for a general graph G we have:

Proposition 2.1.

$$M_1 = \frac{1}{2}\left[\sum_{i=1}^{n}(A^4)_{ii} + 2m\right] - 4q \tag{2}$$

where q is the number of quadrangles in G.

Proof. A result equivalent to Proposition 2.1 was reported already in the early paper [1]. We, nevertheless, re-state its proof.

Let q_i denote the number of quadrangles that contain the vertex i. Note that

$$(A^4)_{ii} = d_i^2 + \sum_{j\sim i} d_j - d_i + 2\,q_i \,.$$

Then

$$\begin{aligned}\sum_{i=1}^{n}(A^4)_{ii} &= \sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n}\sum_{j\sim i} d_j - \sum_{i=1}^{n} d_i + 2\sum_{i=1}^{n} q_i \\ &= M_1(G) + M_1(G) - 2m + 8q \,. \qquad \square\end{aligned}$$

Next we state a few simple relations between the considered indices.

Proposition 2.2. Let G be a connected graph on n vertices. Then,

$$\sqrt{n-1} \leq {}^1R \leq \frac{n}{2} \,.$$

Equality on the left–hand side holds if and only if $G \cong K_{1,n-1}$. Equality on the right–hand side holds holds if and only if G is a regular graph.

Proof. The lower bound is a difficult result, due to Bollobás and Erdős [24]. The upper bound (which holds also for non-connected graphs) has been deduced by several authors (for details see [23]). In what follows we offer another simple proof.

By the arithmetic–geometric inequality,

$$^1R = \sum_{i\sim j} \frac{1}{\sqrt{d_i\,d_j}} \leq \frac{1}{2} \sum_{i\sim j} \left(\frac{1}{d_i} + \frac{1}{d_j} \right) = \frac{1}{2} \sum_{i=1}^{n} \frac{d_i}{d_i} = \frac{n}{2} \; .$$

Clearly, equality holds if and only if $d_i = d_j$ for all pairs of vertices, i. e., if the graph is regular. □

Proposition 2.3.

$$^mM_2 \geq \frac{1}{m}\,(^1R)^2 \geq \frac{n-1}{m}$$

where the left equality holds if and only if G is regular or $K_{1,n-1}$, while the right equality holds if and only if $G \cong K_{1,n-1}$.

Proof.

$$\begin{aligned} ^mM_2 &= \sum_{i\sim j} \left(\frac{1}{\sqrt{d_i\,d_j}} \right)^2 \geq \frac{1}{m} \left(\sum_{i\sim j} \frac{1}{\sqrt{d_i\,d_j}} \right)^2 \qquad \text{(Cauchy inequality)} \\ &= \frac{1}{m}\,(^1R)^2 \geq \frac{n-1}{m} \; . \end{aligned}$$

The first equality holds if and only if $d_i\,d_j = d_\alpha\,d_\beta$ for $i \sim j$, $\alpha \sim \beta$, i. e., if G is either regular or isomorphic to $K_{1,n-1}$. The second equality holds if and only if G is $K_{1,n-1}$. □

Proposition 2.4.

$$\frac{1}{n}\,(^0R)^2 \leq {}^mA \leq \sqrt{n \cdot {}^mM_1}$$

with equality holding if and only if G is a regular graph.

Proof.

$$^mA = \sum_{i=1}^{n} \left(\frac{1}{\sqrt{d_i}} \right)^2 \geq \frac{1}{n} \left(\sum_{i=1}^{n} \frac{1}{\sqrt{d_i}} \right)^2 = \frac{1}{n}\,(^0R)^2 \tag{3}$$

$$^mM_1 = \sum_{i=1}^{n} \left(\frac{1}{d_i} \right)^2 \geq \frac{1}{n} \left(\sum_{i=1}^{n} \frac{1}{d_i} \right)^2 = \frac{1}{n}\,(^mA)^2 \; . \tag{4}$$

The equality in (3) (or (4)) holds if and only if d_i is a constant. □

Proposition 2.5.

$$ {}^{m}A \geq \sqrt{{}^{m}M_1 + 2 \cdot {}^{m}M_2} \qquad \text{and} \qquad {}^{0}R \geq \sqrt{{}^{m}A + 2 \cdot {}^{1}R}\,. $$

Equality holds if and only if $G \cong K_n$.

Proof.

$$ \begin{aligned} ({}^{m}A)^2 &= \left(\sum_i \frac{1}{d_i} \right)^2 = \sum_{i=1}^{n} \frac{1}{d_i^2} + 2 \sum_{i<j} \frac{1}{d_i\, d_j} \ \geq\ {}^{m}M_1 + 2 \sum_{i \sim j} \frac{1}{d_i\, d_j} \\ &= {}^{m}M_1 + 2 \cdot {}^{m}M_2 \end{aligned} $$

since

$$ \sum_{i<j} \frac{1}{d_i\, d_j} = \sum_{i \sim j} \frac{1}{d_i\, d_j} $$

holds if and only if $G \cong K_n$. The other inequality in Proposition 2.5 is deduced in an analogous manner. □

Let $\prod_{i=1}^{n} d_i = D_n$. Then we have:

Proposition 2.6.

$$ \begin{aligned} {}^{m}A &\geq \sqrt{{}^{m}M_1 + n(n-1) \cdot D_n^{-2/n}} \\ {}^{0}R &\geq \sqrt{{}^{m}A + n(n-1) \cdot D_n^{-\frac{1}{n}}}\,. \end{aligned} $$

Equality holds if and only if G is a regular graph.

Proof.

$$ ({}^{m}A)^2 = \left(\sum_{i=1}^{n} \frac{1}{d_i} \right)^2 = \sum_{i=1}^{n} \frac{1}{d_i^2} + 2 \sum_{i<j} \frac{1}{d_i\, d_j}\,. $$

By the arithmetic–geometric inequality,

$$ \frac{2}{n(n-1)} \sum_{i<j} \frac{1}{d_i\, d_j} \geq \left[\prod_{i=1}^{n} \left(\frac{1}{d_i} \right)^{n-1} \right]^{2/[n(n-1)]} = \left(\prod_{i=1}^{n} \frac{1}{d_i} \right)^{2/n} = D_n^{-2/n} $$

with equality holding if and only if $1/(d_i\, d_j)$ is a constant for all i, j, i. e., if G is regular. Thus

$$ {}^{m}A \geq \sqrt{{}^{m}M_1 + n(n-1) \cdot D_n^{-\frac{2}{n}}} $$

and the equality holds if and only if G is regular. Similarly, from

$$({}^0R)^2 = \left(\sum_{i=1}^{n} \frac{1}{\sqrt{d_i}}\right)^2 = \sum_{i=1}^{n} \frac{1}{d_i} + 2\sum_{i<j} \frac{1}{\sqrt{d_i\, d_j}}$$

follows that

$${}^0R \geq \sqrt{{}^mA + n(n-1) \cdot D_n^{-1/n}}\ .$$

Equality holds if and only if G is regular. $\square$

Let

$$\begin{aligned} A(a) &= \frac{1}{n}\sum_{k=1}^{n} a_k && \text{(the arithmetic mean)} \\ H(a) &= n\left(\sum_{k=1}^{n} \frac{1}{a_k}\right) && \text{(the harmonic mean)} \\ G(a) &= \left(\prod_{i=1}^{n} a_i\right)^{1/n} && \text{(the geometric mean)} \end{aligned}$$

where $a_1, a_2, \ldots, a_n$ are positive real numbers.

By the well known inequality

$$1 < \frac{A(a) - H(a)}{A(a) - G(a)} < n$$

we have the following:

Proposition 2.7.

$$n\, D_n^{-1/n} < {}^mA < \frac{n^2}{n^2\, D_n^{1/2} - 2(n-1)m}\ .$$

By the Sierpiński inequality

$$(A(a))^{n-1}\, H(a) \geq (G(a))^n \geq A(a)\, (H(a))^{n-1} \quad (n \geq 2)$$

we have:

Proposition 2.8. For $n \geq 2$,

$$n\left(\frac{n}{2m}\, D_n\right)^{-1/(n-1)} \leq {}^mA \leq \left(\frac{2m}{n}\right)^{n-1} \frac{n}{D_n}\ .$$

3. ESTIMATING THE GENERAL RADIĆ INDEX

We now consider the general cases. Namely we estimate $R_\alpha(G)$ and $Q_\alpha(G)$ for any real number α. There are numerous known estimates of this kind; for details see the book [23] and the newest papers [25–31].

Recalling the Jensen inequality

$$\left(\sum_{k=1}^{n} a_k^s\right)^{1/s} \leq \left(\sum_{k=1}^{n} a_k^r\right)^{1/r}$$

for $0 < r < s$, where $a_1, a_2, \ldots, a_n$ are positive real numbers, we have:

Proposition 3.1. For any real number $\alpha > 1$,

$$R_\alpha(G) \leq M_2^\alpha \ .$$

Proof. By the Jensen inequality,

$$\left(\sum_{i\sim j}(d_i\, d_j)^\alpha\right)^{1/\alpha} \leq \sum_{i\sim j} d_i\, d_j \ . \qquad \square$$

Proposition 3.2. For any real number α,

$$Q_\alpha(G) \geq 2\, R_{(\alpha-1)/2}(G) \ .$$

Equality holds if and only if $\alpha = 1$ or G is regular.

Proof.

$$\begin{aligned} Q_\alpha(G) &= \sum_{i=1}^{n} d_i^\alpha = \sum_{i\sim j}\left(d_i^{\alpha-1} + d_j^{\alpha-1}\right) \\ &\geq 2\sum_{i\sim j}\sqrt{d_i^{\alpha-1}\, d_j^{\alpha-1}} \qquad \text{(arithmetic–geometric inequality)} \\ &= 2\sum_{i\sim j}(d_i\, d_j)^{(\alpha-1)/2} = 2\, R_{(\alpha-1)/2}(G) \ . \end{aligned}$$

Equality holds if and only if $d_i^{\alpha-1} = d_j^{\alpha-1}$, i. e., if either $\alpha = 1$ or G is regular. $\square$

Proposition 3.3. For integral $\alpha \geq 1$,

$$Q_\alpha(G) \leq m(m+1)^{\alpha-1} \ .$$

For a connected graph G, the above equality holds if and only if $\alpha = 2$ and $G \cong K_{1,n-1}$.

Proof.

$$\begin{aligned} Q_\alpha(G) &= \sum_{i=1}^{n} d_i^\alpha = \sum_{i\sim j}(d_i^{\alpha-1} + d_j^{\alpha-1}) \\ &\leq \sum_{i\sim j}(d_i + d_j)^{\alpha-1} \leq \sum_{i\sim j}(m+1)^{\alpha-1} = m(m+1)^{\alpha-1} . \end{aligned}$$

If G is connected, then by Lemma 1 in [17] the above equalities hold if and only if $\alpha = 2$ and $G \cong K_{1,n-1}$. $\square$

Corollary 3.1. For a connected graph G,

$$Q_3(G) \leq m(m+1)^2 - 2\,M_2$$

where the equality holds if and only if $G \cong K_{1,n-1}$.

Proof.

$$\begin{aligned} Q_3(G) &= \sum_{i=1}^{n} d_i^3 = \sum_{i\sim j}(d_i^2 + d_j^2) \\ &= \sum_{i\sim j}(d_i + d_j)^2 - 2\sum_{i\sim j} d_i\, d_j \leq m(m+1)^2 - 2\,M_2 . \end{aligned}$$

By Lemma 1 in [17], the equality holds if and only if $G \cong K_{1,n-1}$. $\square$

Next we will make some estimations for Q_α and R_α in terms of minimum vertex degree δ and maximum vertex degree Δ.

Proposition 3.4. For $\alpha \geq 2$,

$$Q_\alpha \leq 2m\,\delta^{\alpha-1} + (2m - n\,\delta)\sum_{j=0}^{\alpha-2} \Delta^{\alpha-1-j}\,\delta^j .$$

Equality holds if G is of bidegree δ and Δ or regular.

Proof. Let n_i be the number of vertices of degree i in the graph G, $\delta \leq i \leq \Delta$. Thus

$$Q_\alpha = \sum_{i=\delta}^{\Delta} i^\alpha\, n_i \tag{5}$$

where

$$\sum_{i=\delta}^{\Delta} n_i = n \tag{6}$$

$$\sum_{i=\delta}^{\Delta} i \cdot n_i = 2m \ . \tag{7}$$

From (6) and (7) we have

$$n_\delta = \frac{1}{\Delta - \delta} \left[n\Delta - 2m + \sum_{i=\delta+1}^{\Delta-1} (i - \Delta) n_i \right] \tag{8}$$

$$n_\Delta = \frac{1}{\Delta - \delta} \left[2m - n\delta + \sum_{i=\delta+1}^{\Delta-1} (\delta - i) n_i \right] \ . \tag{9}$$

By substituting Eqs. (8) and (9) back into Eq. (5),

$$\begin{aligned}
Q_\alpha &= \frac{1}{\Delta - \delta} \left[\delta^\alpha \left(n\Delta - 2m \right) + \Delta^\alpha \left(2m - n\delta \right) \right] \\
&+ \frac{1}{\Delta - \delta} \sum_{i=\delta+1}^{\Delta-1} \left[\delta^\alpha \left(i - \Delta \right) + i^\alpha \left(\Delta - \delta \right) + \Delta^\alpha \left(\delta - i \right) \right] \, n_i \\
&= (2m - n\delta)(\Delta^{\alpha-1} + \Delta^{\alpha-2} \cdot \delta + \cdots + \Delta \cdot \delta^{\alpha-2}) + 2m \, \delta^{\alpha-1} \\
&+ \sum_{i=\delta+1}^{\Delta-1} \left[(\delta - i) \sum_{j=0}^{\alpha-2} (\Delta^{\alpha-1-j} - i^{\alpha-1-j}) \delta^j \right] \, n_i \\
&= 2m \, \delta^{\alpha-1} + (2m - n\delta) \sum_{j=0}^{\alpha-2} \Delta^{\alpha-1-j} \, \delta^j \\
&+ \sum_{i=\delta+1}^{\Delta-1} (\delta - i) \, n_i \sum_{j=0}^{\alpha-2} (\Delta^{\alpha-1-j} - i^{\alpha-1-j}) \, \delta^j \ .
\end{aligned}$$

Observe that $\delta - i < 0$, $\Delta^{\alpha-1-j} - i^{\alpha-1-j} > 0$ for $\delta + 1 \le i \le \Delta - 1$, and $\alpha \ge 2$. Thus

$$Q_\alpha \le 2m \, \delta^{\alpha-1} + (2m - n\,\delta) \sum_{j=0}^{\alpha-2} \Delta^{\alpha-1-j} \ \delta^j \ .$$

Clearly the equation holds if $n_i = 0$ for $i = \delta + 1, \ldots, \Delta - 1$, i. e., if G has vertices of degree only δ and Δ, or if G is regular. $\square$

Proposition 3.5. For $\alpha > 0$,

$$R_\alpha(G) \leq \frac{1}{2}\, Q_\alpha \left[\left(1 - \frac{1}{n}\right) Q_\alpha + (\Delta - n - 1)\delta^\alpha \right] .$$

Equality holds if and only if G is regular.

Proof.

$$\begin{aligned}
R_\alpha(G) &= \sum_{i\sim j} (d_i\, d_j)^\alpha = \frac{1}{2} \sum_{i=1}^{n} d_i^\alpha \sum_{j\sim i} d_j^\alpha \\
&\leq \frac{1}{2} \sum_{i=1}^{n} d_i^\alpha \left(\sum_{i=1}^{n} d_i^\alpha - d_i^\alpha - (n-1-d_i)\delta^\alpha \right) \qquad (\alpha > 0) && (10) \\
&= \frac{1}{2} \left[\left(\sum_{i=1}^{n} d_i^\alpha \right)^2 - \sum_{i=1}^{n} d_i^{2\alpha} + \delta^\alpha \sum_{i=1}^{n} d_i^{\alpha+1} - (n-1)\,\delta^\alpha \sum_{i=1}^{n} d_i^\alpha \right] && (11) \\
&\leq \frac{1}{2} \left(Q_\alpha^2 - (n-1)\delta^\alpha\, Q_\alpha + \delta^\alpha\, \Delta \cdot Q_\alpha - \sum_{i=1}^{n} d_i^{2\alpha} \right) \\
&\leq \frac{1}{2} \left(Q_\alpha^2 - (n-1)\delta^\alpha\, Q_\alpha + \delta^\alpha\, \Delta \cdot Q_\alpha - \frac{1}{n}\, Q_\alpha^2 \right) \qquad \text{(Cauchy inequality)} \\
&= \frac{1}{2}\, Q_\alpha \left[\left(1 - \frac{1}{n}\right) Q_\alpha + (\Delta - n + 1)\delta^\alpha \right] .
\end{aligned}$$

Clearly all equalities hold if and only if d_i is constant. $\square$

Combing Propositions 3.4 and 3.5 we get:

Corollary 3.2. For $\alpha \geq 2$,

$$\begin{aligned}
R_\alpha &\leq \frac{1}{2} \left(2m\delta^{\alpha-1} + (2m - n\delta) \sum_{j=0}^{\alpha-2} \Delta^{\alpha-1-j} \delta^j \right) \\
&\times \left[2\left(1 - \frac{1}{n}\right) m\delta^{\alpha-1} + \left(1 - \frac{1}{n}\right)(2m - n\delta) \sum_{j=0}^{\alpha-2} \Delta^{\alpha-1-j}\, \delta^j + (\Delta - n + 1)\,\delta^\alpha \right] .
\end{aligned}$$

From formula (11) in Proposition 3.5, we deduce:

Corollary 3.3. For $\alpha > 0$,

$$R_\alpha(G) \leq \frac{1}{2} \left(Q_\alpha^2 - (n-1)\delta^\alpha\, Q_\alpha + \delta^\alpha\, Q_{\alpha+1} - Q_{2\alpha} \right) .$$

In particular, for $\alpha = 1$ (see [16])

$$M_2 \le 2m^2 - (n-1)m\,\delta + \frac{1}{2}\,(\delta - 1)\,M_1\ .$$

Similarly, for $\alpha > 0$ we can estimate $R_\alpha(G)$ from below:

Proposition 3.6. For $\alpha > 0$,

$$R_\alpha(G) \ge \frac{1}{2}\,Q_\alpha \left[\frac{1}{4n}\left(4n - (n-1)^\alpha - \frac{1}{(n-1)^\alpha} - 2\right) Q_\alpha + (\delta - n + 1)\Delta^\alpha\right]\ .$$

Proof.

$$\begin{aligned}
R_\alpha(G) &= \sum_{i\sim j}(d_i\,d_j)^\alpha = \frac{1}{2}\sum_{i=1}^{n} d_i^\alpha \sum_{j\sim i} d_j^\alpha \\
&\ge \frac{1}{2}\sum_{i=1}^{n} d_i^\alpha \left(\sum_{i=1}^{n} d_i^\alpha - d_i^\alpha - (n-1-d_i)\,\Delta^\alpha\right) \\
&= \frac{1}{2}\left[\left(\sum_{i=1}^{n} d_i^\alpha\right)^2 - \sum_{i=1}^{n} d_i^{2\alpha} + \Delta^\alpha \sum_{i=1}^{n} d_i^{\alpha+1} - (n-1)\,\Delta^\alpha \sum_{i=1}^{n} d_i^\alpha\right] \qquad (12) \\
&\ge \frac{1}{2}\left(Q_\alpha^2 - (n-1)\Delta^\alpha\,Q_\alpha + \Delta^\alpha\,\delta\,Q_\alpha - \sum_{i=1}^{n} d_i^{2\alpha}\right)\ .
\end{aligned}$$

We use the Pólya–Szegö inequality as follows. Let $0 < m_1 \le a_k \le M_1$, $0 < m_2 \le b_k \le M_2$ $(k = 1, 2, \ldots, n)$. Then

$$\left(\sum_{k=1}^{n} a_k^2\right)\left(\sum_{k=1}^{n} b_k^2\right) \le \frac{1}{4}\left(\sqrt{\frac{M_1 M_2}{m_1 m_2}} + \sqrt{\frac{m_1 m_2}{M_1 M_2}}\right)^2 \left(\sum_{k=1}^{n} a_k b_k\right)^2$$

since $0 < 1 \le d_i^\alpha \le (n-1)^\alpha$.

Let $b_k = 1$. Then

$$\begin{aligned}
\sum_{i=1}^{n} d_i^{2\alpha} &\le \frac{1}{4n}\left(\sqrt{(n-1)^\alpha} + \sqrt{\frac{1}{(n-1)^\alpha}}\right)^2 \left(\sum_{i=1}^{n} d_i^\alpha\right)^2 \\
&= \frac{1}{4n}\left((n-1)^\alpha + \frac{1}{(n-1)^\alpha} + 2\right) Q_\alpha^2\ .
\end{aligned}$$

Thus

$$\begin{aligned}
R_\alpha(G) &\ge \frac{1}{2}\Big[Q_\alpha^2 - (n-1)\,\Delta^\alpha\,Q_\alpha + \Delta^\alpha\,\delta\,Q_\alpha \\
&- \frac{1}{4n}\left((n-1)^\alpha + \frac{1}{(n-1)^\alpha} + 2\right) Q_\alpha^2\Big] \\
&= \frac{1}{2}\,Q_\alpha\left[\frac{1}{4n}\left(4n - (n-1)^\alpha - \frac{1}{(n-1)^\alpha} - 2\right) Q_\alpha + (\delta - n + 1)\,\Delta^\alpha\right]
\end{aligned}$$

from which Proposition 3.6 follows. □

From formula (12) in Proposition 3.6, we obtain

Corollary 3.4. For $\alpha > 0$,

$$R_\alpha(G) \geq \frac{1}{2}\left[Q_\alpha^2 - (n-1)\Delta^\alpha\, Q_\alpha + \Delta^\alpha\, Q_{\alpha+1} - Q_{2\alpha}\right] .$$

Bearing in mind that ${}^mM_2 = R_{-1}$ and ${}^1R = R_{-1/2}$, we consider $R_\alpha(G)$ for $\alpha < 0$. Note that

$$\sum_{j\in N(i)} d_j^\alpha \leq \sum_{i=1}^{n} d_i^\alpha - d_i^\alpha - (n-1-d_i)\,\Delta^\alpha$$

for $\alpha < 0$. From inequality (10) in Proposition 3.5, we have

$$R_\alpha(G) \leq \frac{1}{2}\sum_{i=1}^{n} d_i^\alpha \left[\sum_{i=1}^{n} d_i^\alpha - d_i^\alpha - (n-1-d_i)\,\Delta^\alpha\right] \;(\alpha < 0) .$$

Thus similar as in Proposition 3.5, we have:

Proposition 3.7. For $\alpha < 0$,

$$\begin{aligned} R_\alpha(G) &\leq \frac{1}{2}\left[Q_\alpha^2 - (n-1)\Delta^\alpha\, Q_\alpha + \Delta^\alpha\, Q_{\alpha+1} - Q_{2\alpha}\right] \\ &\leq \frac{1}{2}\, Q_\alpha \left[\left(1 - \frac{1}{n}\right) Q_\alpha + (\Delta - n + 1)\,\Delta^\alpha\right] . \end{aligned}$$

Setting $\alpha = -1$ or $\alpha = -1/2$ in Proposition 3.7, we have:

Corollary 3.5. For $\alpha = -1$ or $\alpha = -1/2$,

$$\begin{aligned} {}^mM_2 &= R_{-1}(G) \leq \frac{1}{2}\left[({}^mA)^2 - (n-1)\Delta^{-1}\cdot {}^mA + \Delta^{-1} n - {}^mM_1\right] \\ {}^1R &= R_{-1/2}(G) \leq \frac{1}{2}\left[({}^0R)^2 - (n-1)\Delta^{-1/2}\cdot {}^0R + \Delta^{-1/2}\sqrt{2mn} - {}^mA\right] . \end{aligned}$$

Similarly, from Proposition 3.6 we obtain

Proposition 3.8. For $\alpha < 0$,

$$\begin{aligned} R_\alpha(G) &\geq \frac{1}{2}\left[Q_\alpha^2 - (n-1)\delta^\alpha\, Q_\alpha + \delta^\alpha\, Q_{\alpha+1} - Q_{2\alpha}\right] \\ &\geq \frac{1}{2}\, Q_\alpha \left[\frac{1}{4n}\left(4n - (n-1)^\alpha - \frac{1}{(n-1)^\alpha} - 2\right) Q_\alpha + (\delta - n + 1)\,\delta^\alpha\right] . \end{aligned}$$

Corollary 3.6. For $\alpha = -1$ or $\alpha = -1/2$,

$$\begin{aligned} {}^{m}M_2 &= R_{-1}(G) \geq \frac{1}{2}\left[({}^{m}A)^2 - (n-1)\delta^{-1}\cdot {}^{m}A + \delta^{-1}n - {}^{m}M_1\right] \\ {}^{1}R &= R_{-1/2}(G) \geq \frac{1}{2}\,{}^{0}R\left[\frac{1}{4n}\left(4n - \frac{1}{\sqrt{n-1}} - \sqrt{n-1} + -2\right){}^{0}R + \frac{\delta - n + 1}{\sqrt{\delta}}\right] . \end{aligned}$$

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References

[1] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[2] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, *J. Chem. Phys.* **62** (1975) 3399–3405.

[3] A. T. Balaban, I. Motoc, D. Bonchev, O. Mekenyan, Topological indices for structure–activity correlations, *Topics Curr. Chem.* **114** (1983) 21–55.

[4] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.

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

[6] I. Gutman, K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput.Chem.* **50** (2004) 83–92.

[7] S. Nikolić, I. M. Tolić, N. Trinajstić, I. Baučić, On the Zagreb indices as complexity indices, *Croat. Chem. Acta* **73** (2000) 909–921.

[8] I. Gutman, D. Vidović, Two early branching indices and the relation between them, *Theor. Chem. Acc.* **108** (2002) 98–102.

[9] D. Vukičević, A. Graovac, Which valence connectivities realize monocyclic molecules: General algorithm and its application to dest discriminative properties of the Zagreb and modified Zagreb indices, *Croat. Chem. Acta* **77** (2004) 481–490.

[10] D. Vukičević, A. Graovac, Valence connectivities versus Randić, Zagreb and modified Zagreb index: A linear algorithm to check discriminative properties of indices in acyclic molecular graphs, *Croat. Chem. Acta* **77** (2004) 501–508.

[11] D. Vukičević, N. Trinajstić, On the discriminatory power of the Zagreb indices for molecular graphs, *MATCH Commun. Math. Comput. Chem.* **53** (2005) 111–138.

[12] K. C. Das, Maximizing the sum of the squares of the degrees of a graph, *Discr. Math.* **285** (2004) 57–66.

[13] K. C. Das, I. Gutman, Some properties of the second Zagreb index, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 103–112.

[14] B. Zhou, Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 113–118.

[15] I. Gutman, B. Furtula, A. A. Toropov, A. P. Toropova, The graph of atomic orbitals and its basic properties. 2. Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **53** (2005) 225–230.

[16] B. Zhou, I. Gutman, Further properties of Zagreb indices, *MATCH Commum. Math. Comput. Chem.* **54** (2005) 233–239.

[17] B. Liu, I. Gutman, Upper bounds for Zagreb indices of connected graphs, *MATCH Commum. Math. Comput. Chem.* **55** (2006) 439–446.

[18] B. Zhou, D. Stevanović, A note on Zagreb indices, MATCH Commun. Math. Comput. Chem. 56 (2006) 571–578.

[19] D. Vukičević, N. Trinajstić, Modified Zagreb M_2 index – comparison with the Randić connectivity index for benzenoid systems, *Croat. Chem. Acta* **76** (2003) 183–187.

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

[21] H. Zhang, S. Zhang, Unicyclic graphs with the first three smallest and largest first general first Zagreb index, *MATCH. Commun. Math. Comput. Chem.* **55** (2006) 427–438.

[22] S. Zhang, W. Wang, T. C. E. Cheng, Bicyclic graphs with the first three smallest and largest values of the first general Zagreb index, *MATCH Commun. Math. Comput. Chem.* **56** (2006) 579–592.

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

[24] B. Bollobás, P. Erdős, Graphs of extremal weights, *Ars Combin.* **50** (1998) 225–233.

[25] X. Li, J. Zheng, Extremal chemical trees with minimum or maximum Randić index, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 381–390.

[26] X. Li, L. Wang, Y. Zhang, Complete solution for unicyclic graphs with minimum general Randić index, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 391–408.

[27] X. Pan, J. Xu, C. Yang, On the Randić index of unicyclic graphs with k pendent vertices, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 409–417.

[28] Y. Hu, Y. Jin, X. Li, L. Wang, Maximum tree and maximum value for the Randić index R_{-1} of trees of order $n \leq 102$, *MATCH Commun. Math. Comput. Chem.* **56** (2006) 119–136.

[29] L. Pavlović, M. Stojanović, Comment on "Solutions to two unsolved questions on the best upper bound for the Randić index R_{-1}, *MATCH Commun. Math. Comput. Chem.* **56** (2006) 409–414.

[30] M. Aouchiche, P. Hansen, M. Zheng, Variable neighborhood search for extremal graphs 18. Conjectures and results about the Randić index, *MATCH Commun. Math. Comput. Chem.* **56** (2006) 541–550.

[31] X. Li, Y. Shi, T. Xu, Unicyclic graphs with maximum general Randić index for $\alpha > 0$, *MATCH Commun. Math. Comput. Chem.* **56** (2006) 557–570.