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New bounds for Randic and GA indices

V Lokesha[1], B Shwetha Shetty[2], PS Ranjini[3], Ismail Naci Cangul[4*] and Ahmet Sinan Cevik[5]

Dedicated to Professor Hari M Srivastava.

*Correspondence:
cangul@uludag.edu.tr
[4]Department of Mathematics, Faculty of Arts and Science, Uludag University, Gorukle Campus, Bursa, 16059, Turkey
Full list of author information is available at the end of the article

Abstract

The main goal of this paper is to present some new lower and upper bounds for the Randic and GA indices in terms of Zagreb and modified Zagreb indices.

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1 Introduction and preliminaries

A systematic study of *topological indices* is one of the most striking aspects in many branches of mathematics with its applications and various other fields of science and technology. A topological index is a numeric quantity from the structural graph of a molecule. Usage of topological indices in chemistry began in 1947 when H. Wiener developed the most widely known topological descriptor, namely the Wiener index, and used it to determine physical properties of types of alkanes known as paraffin (see, for instance, [1–3]).

Let G be a simple graph with the vertex-set $V(G)$ and the edge-set $E(G)$. As usual notion, the maximum vertex degree is denoted by $\Delta = \Delta(G)$, while the minimum vertex degree is denoted by $\delta = \delta(G)$. Moreover, $\delta_1 = \delta_1(G)$ denotes the minimum nonpendant vertex degree in G. A vertex of the graph G is said to be *pendant* if its neighborhood contains exactly one vertex. On the other hand, an edge of a graph is said to be *pendant* if one of its vertices is pendant.

In 1975, Randic [4] introduced the connectivity index, namely *Randic index*, to reflect molecular branching. In fact, the Randic index is defined as

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

Furthermore, again by considering the degrees of vertices in G, Vukicević and Furtula [5] developed the *Geometric-arithmetic index*, shortly GA index, which is defined by

$$\mathrm{GA}(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}. \tag{2}$$

In the following, we recall two fundamental indices that will be used to present some new bounds for Randic and GA indices.

The (first and second) *Zagreb indices* have been introduced by Gutman and Trinajstić [6] as the form

$$M_1(G) = \sum_{v \in V(G)} (d_v)^2 \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d_u d_v, \tag{3}$$

where d_u and d_v are the *degrees* of u and v, respectively. On the other hand, for a (molecular) graph G, the *modified second Zagreb index* $M_2^*(G)$ is defined as

$$M_2^*(G) = \sum_{uv \in E(G)} \frac{1}{d_u d_v} \tag{4}$$

(*cf.* [7–10]).

This paper is organized as follows. In the forthcoming section, we present lower and upper bounds on Randic index of connected graphs and trees in terms of modified Zagreb indices given in (4). The final section deals with lower and upper bounds on GA index of connected graphs and trees in terms of Zagreb indices given in (3). We note that this paper is motivated from [11].

2 Lower and upper bounds on Randic index

Throughout this paper, we refer the book [12] for a classical result, namely the *Pólya-Szegó inequality*. From this result, we first establish the following theorem, which will be expressed the lower bound on the Randic index.

Theorem 1 *Let G be a simple connected graph of order n with m edges, and let p, Δ and δ_1 denote the number of pendant vertices, maximum vertex degree and minimum nonpendant vertex degree of G, respectively. Then*

$$\chi(G) \ge \frac{p}{\sqrt{\Delta}} + \frac{2\sqrt{\delta_1 \Delta (m-p)}}{\delta_1 + \Delta} \sqrt{M_2^*(G) - \frac{p}{\Delta}}.$$

Proof For $2 \le \delta_1 \le d_i, d_j \le \Delta$, we clearly have

$$\frac{1}{d_i d_j} \ge \frac{1}{d_i \Delta} \ge \frac{1}{\Delta^2}$$

such that the equality holds if and only if $d_i = d_j = \Delta$. We also have

$$\frac{1}{d_i d_j} \le \frac{1}{d_i \delta_1} \le \frac{1}{\delta_1^2}$$

with equality holding if and only if $d_i = d_j = \delta_1$.

Since p is the number of pendant vertices in G, we have total $m-p$ number of non-pendant edges in G. By the Pólya-Szegó inequality, we have

$$\begin{aligned}\left(\sum_{v_i v_j \in E(G): d_j, d_j \neq 1} \frac{1}{\sqrt{d_i d_j}}\right)^2 &\ge \frac{4\delta_1 \Delta (m-p)}{(\delta_1 + \Delta)^2} \left(\sum_{v_i v_j \in E(G): d_i, d_j \neq 1} \frac{1}{d_i d_j}\right) \\ &\ge \frac{4\delta_1 \Delta (m-p)}{(\delta_1 + \Delta)^2} \left(M_2^*(G) - \sum_{v_i v_j \in E(G): d_i = 1} \frac{1}{d_j}\right).\end{aligned}$$

This inequality can be clearly written as

$$\sum_{v_iv_j\in E(G):d_j,d_j\neq 1}\frac{1}{\sqrt{d_id_j}}\geq\frac{\sqrt{4\delta_1\Delta(m-p)}}{(\delta_1+\Delta)}\sqrt{M_2^*(G)-p\frac{1}{\Delta}}.\tag{5}$$

From (1), we get

$$\chi(G)=\sum_{v_iv_j\in E(G):d_i=1}\frac{1}{\sqrt{d_j}}+\sum_{v_iv_j\in E(G):d_i,d_j\neq 1}\frac{1}{\sqrt{d_id_j}}.\tag{6}$$

For $\Delta\geq d_i$, since $\frac{1}{d_i}\geq\frac{1}{\Delta}$, by (5) and (6), we obtain

$$\chi(G)\geq\frac{p}{\sqrt{\Delta}}+\frac{2\sqrt{\delta_1\Delta(m-p)}}{\delta_1+\Delta}\sqrt{M_2^*(G)-\frac{p}{\Delta}},$$

as desired. □

Corollary 1 *Let T be a tree of order n with p pendant vertices, and let Δ and δ_1 be the maximum vertex and minimum nonpendent vertex degrees of T, respectively. Then*

$$\chi(T)\geq\frac{p}{\sqrt{\Delta}}+\frac{2\sqrt{\delta_1\Delta(n-1-p)}}{\delta_1+\Delta}\sqrt{M_2^*(G)-\frac{p}{\Delta}}.$$

Proof Since the number of edges in a tree having n vertices is $m=n-1$, the proof can be done similarly as in the proof of Theorem 1. □

Theorem 2 *Let G be a simple connected graph of order n with m edges, and let p, Δ and δ_1 denote the number of pendant vertices, maximum vertex degree and minimum nonpendant vertex degree of G, respectively. Then*

$$\chi(G)\leq\frac{p}{\sqrt{\delta_1}}+\sqrt{(m-p)\left(M_2^*(G)-\frac{p}{\delta_1}\right)}.$$

Proof By the Cauchy-Schwarz inequality, it is clear that

$$\begin{aligned}\left(\sum_{v_iv_j\in E(G):d_j,d_j\neq 1}\frac{1}{\sqrt{d_id_j}}\right)^2&\leq(m-p)\left(\sum_{v_iv_j\in E(G):d_j,d_j\neq 1}\frac{1}{d_id_j}\right)\\&\leq(m-p)\left(M_2^*(G)-\sum_{v_iv_j\in E(G):d_i=1}\frac{1}{d_j}\right)\\&\leq(m-p)\left(M_2^*(G)-\frac{p}{\delta_1}\right)\end{aligned}$$

which can be rewritten as

$$\sum_{v_iv_j\in E(G):d_j,d_j\neq 1}\frac{1}{\sqrt{d_id_j}}\leq\sqrt{(m-p)\left(M_2^*(G)-\frac{p}{\delta_1}\right)}.\tag{7}$$

Since $\frac{1}{d_j} \le \frac{1}{\delta_1}$ for $\delta_1 \le d_j$, by (5) and (7), we obtain

$$\chi(G) \le \frac{p}{\sqrt{\delta_1}} + \sqrt{(m-p)\left(M_2^*(G) - \frac{p}{\delta_1}\right)},$$

as required. □

Now we prove another form of the upper bound for the Randic index as in the following.

Theorem 3 *Let G be a simple connected graph of order n with m edges, and let p, Δ and δ_1 denote the number of pendant vertices, maximum vertex degree and minimum nonpendant vertex degree of G, respectively. Then*

$$\chi(G) \le \frac{p}{\sqrt{\delta_1}} + \frac{(m-p)}{\delta_1}. \tag{8}$$

Proof Since $\frac{1}{\delta_1^2}$ is the maximum value of $\frac{1}{d_i d_j}$ for all edges $v_i v_j \in E(G)$, we have

$$\begin{aligned} M_2^*(G) - \sum_{v_i v_j \in E(G): d_i = 1} \frac{1}{d_j} &= \sum_{v_i v_j \in E(G): d_j, d_j \neq 1} \frac{1}{\sqrt{d_i d_j}} \\ &\le \frac{m-p}{\delta_1^2}. \end{aligned} \tag{9}$$

After that, by using (9) in (5), we get the bound in (8), as required. □

3 Lower and upper bounds on GA index

By taking Pólya-Szegó inequality into account, the next result deals with a new lower bound on GA index in terms of Zagreb index as given in (3).

Theorem 4 *Let G be a simple connected graph of order n with m edges, and let p, Δ and δ_1 denote the number of pendant vertices, maximum vertex degree and minimum nonpendant vertex degree of G, respectively. Then*

$$\mathrm{GA}(G) \ge \frac{2p\sqrt{\delta_1}}{1+\Delta} + 2\sqrt{2}\frac{\delta_1 \Delta}{(\delta_1^2 + \Delta^2)} \sqrt{\frac{(m-p)}{\Delta}\big(M_2(G) - p\delta_1\big)}.$$

Proof For $2 \le \delta_1 \le d_i, d_j \le \Delta$, we have

$$\frac{1}{2\Delta} \le \frac{1}{(d_i + d_j)} \le \frac{1}{2\delta_1}$$

which implies

$$\frac{d_i d_j}{(d_i + d_j)^2} \le \frac{\Delta^2}{4\delta_1^2}.$$

On the other hand, since we also have

$$\frac{d_i d_j}{(d_i + d_j)^2} \ge \frac{\delta_1^2}{4\Delta^2},$$

the combination of these above equalities implies that

$$\frac{\delta_1}{\Delta} \le \frac{2\sqrt{d_i d_j}}{(d_i + d_j)} \le \frac{\Delta}{\delta_1}. \tag{10}$$

Since p is the number of pendant vertices in G, we have total $m - p$ number of non-pendant edges in G. By the Pólya-Szegó inequality, we get

$$\begin{aligned}\left(\sum_{v_iv_j\in E(G):d_j,d_j\neq 1} \frac{2\sqrt{d_i d_j}}{(d_i + d_j)}\right)^2 &\ge \frac{4\delta_1^2\Delta^2(m-p)}{(\delta_1^2+\Delta^2)^2}\left(\sum_{v_iv_j\in E(G):d_i,d_j\neq 1} \frac{4d_id_j}{(d_i + d_j)}\right)\\ &\ge \frac{4\delta_1^2\Delta^2(m-p)}{(\delta_1^2+\Delta^2)^2}\left(\sum_{v_iv_j\in E(G):d_i,d_j\neq 1} \frac{4d_id_j}{2\Delta}\right)\\ &\ge \frac{8\delta_1^2\Delta^2(m-p)}{\Delta(\delta_1^2+\Delta^2)^2}\left(M_2(G) - \sum_{v_iv_j\in E(G):d_i=1} d_j\right)\\ &\ge \frac{8\delta_1^2\Delta^2(m-p)}{\Delta(\delta_1^2+\Delta^2)^2}\bigl(M_2(G) - p\delta_1\bigr).\end{aligned}$$

This calculation can be rewritten basically as follows:

$$\sum_{v_iv_j\in E(G):d_j,d_j\neq 1} \frac{2\sqrt{d_i d_j}}{(d_i + d_j)} \ge 2\sqrt{2}\frac{\delta_1\Delta}{(\delta_1^2+\Delta^2)}\sqrt{\frac{(m-p)}{\Delta}\bigl(M_2(G) - p\delta_1\bigr)}.$$

From (2), we obtain

$$\mathrm{GA}(G) = \sum_{v_iv_j\in E(G):d_i=1} \frac{2\sqrt{d_j}}{(1 + d_j)} + \sum_{v_iv_j\in E(G):d_i,d_j\neq 1} \frac{2\sqrt{d_i d_j}}{(d_i + d_j)}. \tag{11}$$

Now, for $\delta_1 \le d_j \le \Delta$, since $\sqrt{d_j} \ge \sqrt{\delta_1}$ and $\frac{1}{1+d_j} \ge \frac{1}{1+\Delta}$, by (10) and (11), we arrive at

$$\mathrm{GA}(G) \ge \frac{2p\sqrt{\delta_1}}{1+\Delta} + 2\sqrt{2}\frac{\delta_1\Delta}{(\delta_1^2+\Delta^2)}\sqrt{\frac{(m-p)}{\Delta}\bigl(M_2(G) - p\delta_1\bigr)}.$$

Hence the result. □

Corollary 2 *Let T be a tree of order n with p pendant vertices, and let Δ and δ_1 denote the maximum vertex degree and minimum non-pendent vertex degree of T, respectively. Then*

$$\mathrm{GA}(G) \ge \frac{2p\sqrt{\delta_1}}{1+\Delta} + 2\sqrt{2}\frac{\delta_1\Delta}{(\delta_1^2+\Delta^2)}\sqrt{\frac{(n-1-p)}{\Delta}\bigl(M_2(G) - p\delta_1\bigr)}.$$

Proof For an order n, since the number of edges in a tree T is $m = n - 1$, the proof can be done quite similar as the proof of Theorem 4. □

Theorem 5 *Let G be a simple connected graph of order n with m edges, and let p, Δ and δ_1 denote the number of pendant vertices, maximum vertex degree and minimum non-*

pendant vertex degree of G, respectively. Then

$$\mathrm{GA}(G) \leq \frac{2p\sqrt{\Delta}}{1+\delta_1} + \frac{1}{\delta_1}\sqrt{(m-p)\bigl(M_2(G) - p\Delta\bigr)}.$$

Proof By the Cauchy-Schwarz inequality,

$$\begin{aligned}\Bigl(\sum_{v_iv_j \in E(G): d_j, d_j \neq 1} \frac{2\sqrt{d_id_j}}{(d_i+d_j)}\Bigr)^2 &\leq (m-p)\Bigl(\sum_{v_iv_j \in E(G): d_j, d_j \neq 1} \frac{4d_id_j}{(d_i+d_j)^2}\Bigr)\\ &\leq (m-p)\Bigl(\sum_{v_iv_j \in E(G): d_j, d_j \neq 1} \frac{d_id_j}{\delta_1^2}\Bigr)\\ &\leq \frac{(m-p)}{\delta_1^2}\Bigl(M_2(G) - \sum_{v_iv_j \in E(G): d_i = 1} d_j\Bigr)\\ &\leq \frac{(m-p)}{\delta_1^2}\bigl(M_2(G) - p\Delta\bigr)\end{aligned}$$

which can be simply indicate as

$$\sum_{v_iv_j \in E(G): d_j, d_j \neq 1} \frac{2\sqrt{d_id_j}}{(d_i+d_j)} \leq \frac{1}{\delta_1}\sqrt{(m-p)\bigl(M_2(G) - p\Delta\bigr)}. \tag{12}$$

Now, for $\delta_1 \leq d_j \leq \Delta$, since $\sqrt{d_j} \leq \sqrt{\Delta}$ and $\frac{1}{1+d_j} \leq \frac{1}{1+\delta_1}$, by (11) and (12) we get the result, as required. □

The following theorem presents another upper bound for GA index.

Theorem 6 *Let G be a simple connected graph of order n with m edges, and let p, Δ and δ_1 denote the number of pendant vertices, maximum vertex degree and minimum non-pendant vertex degree of G, respectively. Then*

$$G(A) \leq \frac{2p\sqrt{\Delta}}{1+\delta_1} + \frac{(m-p)\Delta}{\delta_1}.$$

Proof Since Δ^2 is the maximum value of d_id_j for all edges $v_iv_j \in E(G)$, we have

$$\begin{aligned}M_2(G) - \sum_{v_iv_j \in E(G): d_i = 1} d_j &= \sum_{v_iv_j \in E(G): d_j, d_j \neq 1} d_id_j\\ &\leq (m-p)\Delta^2. \end{aligned} \tag{13}$$

Now, by using (13) in (11), we get

$$G(A) \leq \frac{2p\sqrt{\Delta}}{1+\delta_1} + \frac{(m-p)\Delta}{\delta_1}.$$

Hence, the result. □

Competing interests
The authors declare that they have no competing interests.

Authors' contributions
All authors completed the paper together. All authors read and approved the final manuscript.

Author details
[1]Department of Mathematics, V S K University, Bellary, 583 104, India. [2]Department of Mathematics, Sri Krishna School of Engineering and Management, Bangalore, 35, India. [3]Department of Mathematics, Don Bosco Institute of Technology, Bangalore, 78, India. [4]Department of Mathematics, Faculty of Arts and Science, Uludag University, Gorukle Campus, Bursa, 16059, Turkey. [5]Department of Mathematics, Faculty of Science, Selcuk University, Campus, Konya, 42075, Turkey.

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