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BOUNDS ON RZ-INVARIANT OF GRAPHS

K. Pattabiraman and Manzoor Ahmad Bhat*

Department of Mathematics,
Government Arts College(Autonomous),
Kumbakonam - 612002, Tamil Nadu, INDIA

E-mail : pramank@gmail.com

*Department of Mathematics,
Annamalai University, Annamalai Nagar,
Annamalai Nagar - 608002, Tamil Nadu, INDIA

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Abstract: The RZ-invariant of a simple connected graph G is defined as the sum of the terms $(Deg(u) + Deg(v) - 2)^2$ over all edges uv of G, where $Deg(u)$ is the degree of a vertex u in G. In this paper, we obtain some new upper and lower bounds for the RZ-invariant in terms of other graph parameters.

Keywords and Phrases: Degree, Zagreb invariant, RZ-invariant.

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1. Introduction

Topological index is a graph theoretical property that is preserved by isomorphism. The chemical information derived through *topological index* has been found useful in chemical documentation, isomer discrimination, structure property correlations. The interest in topological indices is mainly related to their use in non-empirical quantitative structure-property relationships and quantitative structural-activity relationships. The first and second Zagreb invariant of a graph were first introduced by Gutman in [4] which are the oldest and most used topological indices [3, 1] defined as $M_1(G) = \sum_{v \in E(G)} Deg(v)^2$ and $M_2(G) = \sum_{uv \in E(G)} Deg(u)Deg(v)$.

Analogues to Zagreb indices Milicević et al. [6] in 2004 reformulated the Zagreb invariant in terms of edge degrees instead of vertex degrees, where the degree of an edge $Deg(e)$ is defined as $Deg(e) = Deg(u) + Deg(v) - 2$. Thus the first RZ-invariant of a graph G is defined as $RZ(G) = \sum_{e \in E(G)} Deg(e)^2 = \sum_{uv \in E(G)} (Deg(u) + Deg(v) - 2)^2$. RZ-invariant, particularly its upper and lower bounds has attracted recently the attention of many mathematicians and computer scientists, see [2, 5, 6, 7]. In this paper, we obtain some new upper and lower bounds for the RZ-invariant in terms of other graph parameters.

2. Main Results

The inverse vertex degree of G, denoted by $ID(G)$, is defined as $ID(G) = \sum_{x \in V(G)} \frac{1}{Deg(x)}$ and the inverse edge degree of G with non-isolated edges is defined as $ID_e(G) = \sum_{e \in E(G)} \frac{1}{Deg(e)}$.

Theorem 2.1. *Let G be a graph with s vertices and t edges. Then $RZ(G) \leq 2\Big(\Delta(G) + \delta(G) - 2\Big)M_1(G) - 4t\Big(\Delta(G)\delta(G) - 1\Big)$ with equality if and only if G is regular.*

Proof. For any vertex $v \in V(G)$, we have $\delta(G) \leq Deg(v) \leq \Delta(G)$. Similarly, for any edge $e_i \in E(G)$, we get $2(\delta(G) - 1) \leq Deg(e) \leq Deg(v) \leq 2(\Delta(G) - 1)$ with the edges are labeled and bounded by $\delta(G) \leq Deg(v_i) \leq \Delta(G)$ for $i = 1, 2 \ldots, s$. The edge degree is bounded by $e_1, e_2, \ldots, e_t$ such that $Deg(e_1) \geq Deg(e_2) \geq \ldots \geq Deg(e_t)$. Hence

$$\sum_{i=1}^{t} Deg(e_i)^2 = \sum_{i=1}^{t} \Big(Deg(e_i)(Deg(e_i) - Deg(e_t)) + Deg(e_i)Deg(e_t)\Big)$$
$$\leq \sum_{i=1}^{t} \Big(Deg(e_1)(Deg(e_i) - Deg(e_t)) + Deg(e_i)Deg(e_t)\Big)$$
$$\leq \sum_{i=1}^{t} \Big(2(\Delta(G) - 1\Big)\Big(Deg(e_i) - 2(\delta(G) - 1)\Big) + Deg(e_i)2\Big(\delta(G) - 1\Big)\Big)$$
$$= \Big(2(\Delta(G) + \delta(G)) - 4\Big)\sum_{i=1}^{t} \Big(Deg(e_i) - 4(\Delta(G) - 1)\Big)\Big(\delta(G) - 1\Big)\sum_{i=1}^{t}(1).$$

From the definition of RZ-invariant, we obtain; $\sum_{uv \in E(G)} \Big(Deg(u) + Deg(v) - 2\Big)^2 \leq \Big(2(\Delta(G) + \delta(G)) - 4\Big) \sum_{uvE(G)} \Big(Deg(u) + Deg(v) - 2\Big) - 4(\delta(G) - 1)(\Delta(G) - 1) \sum_{uv \in E(G)} (1)$. Hence $RZ(G) \leq 2\Big(\Delta(G) + \delta(G) - 2\Big)M_1(G) - 4\Big(\Delta(G)\delta(G) - 1\Big)t$. This completes the proof with equality if and only if G is regular.

Next we improve the bounds given in Theorem 2.1 by using Harmonic index

$H(G)$ which is defined for a connected graph G as $H(G) = \sum\limits_{uv\in E(G)} \frac{2}{Deg(u)+Deg(v)}$.

Theorem 2.2. *Let G be a simple connected graph with s vertices and t edges. Then $RZ(G) \leq \Big(2(\Delta(G)+\delta(G))-3\Big)M_1(G) - 2t\Big(\Delta(G)+\delta(G)+2\delta(G)\Delta(G) - \delta(G)\Delta(G)H(G)-2\Big)$. Equality holds if and only if G is a regular graph.*

Proof. By Theorem 2.1, $RZ(G) \leq 2\Big(\Delta(G)+\delta(G)-2\Big)M_1(G)-4t\Big(\delta(G)\Delta(G)-1\Big)$. For any edge $uv \in E(G)$, it is true that $\frac{1}{Deg(u)+Deg(v)} < 1$ and using in the above inequality, we obtain

$$\sum_{uv\in E(G)} \left[1 - \frac{1}{Deg(u)+Deg(v)}\right]\Big(Deg(u)+Deg(v)-2\Big)^2$$
$$\leq \Big(2(\Delta(G)+\delta(G))-4\Big)\sum_{uv\in E(G)} \left[1-\frac{1}{Deg(u)+Deg(v)}\right]\Big(Deg(u)+Deg(v)\Big)$$
$$-4(\Delta(G)\delta(G)-1)\sum_{uv\in E(G)}\left[1-\frac{1}{Deg(u)+Deg(v)}\right].$$

$$\sum_{uv\in E(G)}\left[\Big(Deg(u)+Deg(v)-2\Big)^2 - \Big(Deg(u)+Deg(v)\Big)+4-\frac{4}{Deg(u)+Deg(v)}\right]$$
$$\leq \Big(2(\Delta(G)+\delta(G))-4\Big)\sum_{uv\in E(G)}[Deg(u)+Deg(v)] - \Big(2(\Delta(G)+\delta(G))-4\Big)t$$
$$-4\Big(\Delta(G)\delta(G)-1\Big)t + \sum_{uv\in E(G)}\left(\frac{4(\Delta(G)\delta(G)-1)}{Deg(u)+Deg(v)}\right).$$

By the definitions of Zagreb and RZ invariants, we have

$$RZ(G) - M_1(G) + 4t - 2H(G) \leq \Big(2(\Delta(G)+\delta(G))-4\Big)M_1(G) - \Big(2(\Delta(G)+\delta(G))-4\Big)t$$
$$-4\Big(\Delta(G)\delta(G)-1\Big)t + 2\Big(\Delta(G)\delta(G)-1\Big)\sum_{uv\in E(G)}\left(\frac{2}{Deg(u)+Deg(v)}\right).$$

Hence $RZ(G) = M_1(G)+2H(G)-4t+\Big(2(\Delta(G)+\delta(G))-4\Big)M_1(G) - 2(\Delta(G)+\delta(G))t + 4t - 4(\Delta(G)\delta(G))t + 4t + 2(\Delta(G)\delta(G)-1)H(G) = \Big(2(\Delta(G)+\delta(G)) - 3\Big)M_1(G) - 2(\Delta(G)+\delta(G))t - 4\Delta(G)\delta(G)t + 4t + 2\Delta(G)\delta(G)H(G)$. Equality holds if and only if G is a regular graph, hence completes the proof.

Theorem 2.3. *Let G be a simple connected graph with s vertices and t edges. If G*

has no isolated edges, then $RZ(G) \leq \Big(2(\Delta(G)+\delta(G))-3\Big)M_1(G) - 2t\Big(3\Delta(G) + 3\delta(G) + 2(\Delta(G)-1)(\delta(G)-1)-5\Big) + 4(\Delta(G)-1)(\delta(G)-1)ID_e(G)$ *with equality if and only G is a regular graph.*

Proof. Let G be a graph with no isolated edges. Then $Deg(u)+Deg(v) > 2$ and with the assumption of the proof of Theorem 2.1, we have

$$\begin{aligned}\sum_{i=1}^{t}\left[1-\frac{1}{Deg(e_i)}\right]Deg(e_i)^2 \quad &\leq \quad \Big(2(\Delta(G)+\delta(G))-4\Big)\sum_{i=1}^{t}\left[1-\frac{1}{Deg(e_i)}\right]Deg(e_i)\\ &\quad -4(\Delta(G)-1)(\delta(G)-1)\sum_{i=1}^{t}\left[1-\frac{1}{Deg(e_i)}\right].\end{aligned}$$

$$\begin{aligned}\sum_{i=1}^{t}Deg(e_i)^2 - \sum_{i=1}^{t}Deg(e_i) \quad &\leq \quad \Big(2(\Delta(G)+\delta(G))-4\Big)\Big[\sum_{i=1}^{t}Deg(e_i) - \sum_{i=1}^{t}1\Big]\\ &\quad -4(\Delta(G)-1)(\delta(G)-1)\Big[\sum_{i=1}^{t}1 + \sum_{i=1}^{t}\frac{1}{Deg(e_i)}\Big].\end{aligned}$$

$$\begin{aligned}\sum_{uv\in E(G)}(Deg(u)+Deg(v)-2)^2 \quad &\leq \quad \sum_{uv\in E(G)}(Deg(u)+Deg(v)-2)\\ &\quad +\Big(2(\Delta(G)+\delta(G))-4\Big)\sum_{uv\in E(G)}(Deg(u)+Deg(v)-2)\\ &\quad -\Big(2(\Delta(G)+\delta(G))-4\Big)t - 4(\Delta(G)-1)(\delta(G)-1)t\\ &\quad +4(\Delta(G)-1)(\delta(G)-1)\sum_{uv\in E(G)}\frac{1}{(Deg(u)+Deg(v)-2)}.\end{aligned}$$

From the definition of RZ-invariant, we have $RZ(G) \leq M_1(G) - 2t + 2\Big(\Delta(G) + \delta(G) - 2\Big)M_1(G) - 6\Big(\Delta(G)+\delta(G)-2\Big)t - 4(\Delta(G)-1)(\delta(G)-1)t + 4(\Delta(G) - 1)(\delta(G)-1)ID_e(G) = \Big(1+2((\Delta(G)+\delta(G))-2)\Big)M_1(G) + 10t - 6(\Delta(G)+\delta(G))t - 4(\Delta(G)-1)(\delta(G)-1)t + 4(\Delta(G)-1)(\delta(G)-1)ID_e(G)$. The equality holds for any vertex $v \in V(G)$, $Deg(v) = \Delta(G) = \delta(G)$. This implies that G is regular.

The bidegreed graph is a graph whose vertices have exactly two vertex degrees $\Delta(G)$ and $\delta(G)$.

Theorem 2.4. *Let G be a simple connected graph with s vertices and t edges. If G has no isolated edges, then* $RZ(G) \leq \Big(\Delta(G)+\delta(G)-4\Big)M_1(G) + \Delta(G)\delta(G)ID(G) - 2t(\Delta(G)\delta(G)-3) - (\Delta(G)+\delta(G))s$ *with equality if and only if G is regular (or)* *bidegreed graph.*

Proof. Suppose $a, A \in R$ and x_i, y_i be two sequences in such a way that it has the property $ay_i \leq x_i \leq Ay_i$ for $i = 1, 2, \dots, s$ and w_i be any sequence of positive real numbers, it holds $w_i(Ay_i - x_i)(x_i - ay_i) \geq 0$. Since w_i is a positive sequence, choose $w_i = m_i - n_i$ such that $m_i \geq n_i$, we get $\sum\limits_{i=1}^{s}(m_i - n_i)\Big((A+a)x_iy_i - x_i^2 - Aay_i^2\Big) \geq 0$. By setting $A = \Delta(G)$,$a = \delta(G), x_i = Deg(v_i), y_i = 1, m_i = Deg(v_i)$ and $n_i = Deg(v_i)^{-1}$, we have

$(\Delta(G) + \delta(G)) \sum\limits_{i=1}^{s} Deg(v_i)^2 - \sum\limits_{i=1}^{s} Deg(v_i)^3 - (\Delta(G)\delta(G)) \sum\limits_{i=1}^{s} Deg(v_i) \geq (\Delta(G) + \delta(G)) \sum\limits_{i=1}^{s} 1 - \sum\limits_{i=1}^{s} Deg(v_i) - (\Delta(G)\delta(G)) \sum\limits_{i=1}^{s} \frac{1}{Deg(v_i)}$. Simplify the above inequality, we have $(\Delta(G)+\delta(G))M_1(G) - F(G) - 2t\Delta\delta \geq (\Delta(G)+\delta(G))s - 2t - \Delta(G)\delta(G)ID(G)$.

$F(G) \leq (\Delta(G)+\delta(G))M_1(G) - 2t\Delta\delta - (\Delta(G)+\delta(G))s + 2t + \Delta(G)\delta(G)ID(G) + 4t - 4M_1(G)$.

From the definition of RZ-invariant, we obtain $RZ(G) \leq (\Delta(G) + \delta(G) - 4)M_1(G) + \Delta(G)\delta(G)ID(G) - 2t(\Delta(G)\delta(G) - 3) - (\Delta(G) + \delta(G))s$.

Theorem 2.5. *Let G be a simple connected graph with s vertices and t edges. If G has no isolated edges, then $RZ(G) \leq \Big(\Delta(G)+\delta(G)-4\Big)M_1(G)+\Delta(G)\delta(G)ID(G)-2t(\delta(G)\delta(G) - 3) - (\delta(G) + \delta(G))s$.*

Proof. The proof follows by using similar arguments as in the proof of theorem **??**. By setting $A = \Delta(G)$,$a = \delta(G), x_i = d(v_i), y_i = 1, t_i = d(v_i)$ and $a_i = 1$, we have $(\Delta(G)+\delta(G)) \sum\limits_{i=1}^{s} Deg(v_i)^2 - \sum\limits_{i=1}^{a} Deg(v_i)^3 - (\Delta(G)\delta(G)) \sum\limits_{i=1}^{s} Deg(v_i) \geq (\Delta(G)+\delta(G)) \sum\limits_{i=1}^{s} Deg(v_i) - \sum\limits_{i=1}^{s} Deg(v_i)^2 - (\Delta(G)\delta(G)) \sum\limits_{i=1}^{s}(1)$.

$(\Delta(G) + \delta(G))M_1(G) - F(G) - 2t\Delta(G)\delta(G) \geq (\Delta(G) + \delta(G))2t + M_1(G) + \Delta(G)\delta(G)s$. $F(G) \leq (\Delta(G) + \delta(G))M_1(G) - 2t\Delta(G)\delta(G) - (\Delta(G) + \delta(G))2t + M_1(G)+\Delta(G)\delta(G)s+4t-4M_1(G)$. From the definition of RZ-invariant, we obtain the required result.

Theorem 2.6. *Let G be a simple connected graph with s vertices and t edges. If G has no isolated edges, then $RZ(G) \geq F(G)+2M_2(G)+4t-4M_1(G)+\frac{1}{2t}[(M_1(G))^2 - s^2] + ID(G)$. Equality holds if and only if G is regular.*

Proof. Suppose $w_1, w_2, \dots, w_n$ be non-negative weights, then we have the weighted version of Cauchy-Schwartz inequality, we have $\sum\limits_{i=1}^{n} w_ia_i^2 \sum\limits_{i=1}^{n} w_ib_i^2 \geq \left(\sum\limits_{i=1}^{n} w_ia_ib_i\right)^2$. Let $w_i = m_i - n_i$ such that $m_i \geq n_i \geq 0$. Then

$$\sum_{i=1}^{s} m_i a_i^2 \sum_{i=1}^{s} m_i b_i^2 - \left(\sum_{i=1}^{s}(m_i a_i b_i)\right)^2 \geq \sum_{i=1}^{s} n_i a_i^2 \sum_{i=1}^{s} n_i b_i^2 - \left(\sum_{i=1}^{s}(n_i a_i b_i)\right)^2 \geq 0.$$

By setting $m_i = Deg(v_i)$, $n_i = \frac{1}{Deg(v_i)}$, $a_i = Deg(v_i)$ and $b_i = 1$, for all $i = 1, 2, \ldots, s$ in the above inequality we have,

$$\sum_{i=1}^{s} Deg(v_i)^3 \sum_{i=1}^{s} Deg(v_i) - \left(\sum_{i=1}^{s} Deg(v_i)^2\right)^2 \geq \sum_{i=1}^{s} Deg(v_i) \sum_{i=1}^{s} \frac{1}{Deg(v_i)} - \left(\sum_{i=1}^{s}(1)\right)^2$$

$$\sum_{i=1}^{n} Deg(v_i)^3 \geq \frac{1}{\sum_{i=1}^{s} Deg(v_i)} \left[\left(\sum_{i=1}^{s} Deg(v_i)^2\right)^2 + \sum_{i=1}^{s} Deg(v_i) \sum_{i=1}^{s} \frac{1}{Deg(v_i)} - \left(\sum_{i=1}^{s}(1)\right)^2\right].$$

Hence $RZ(G) \geq F(G) + 2M_2(G) + 4t - 4M_1(G) + \frac{1}{2m}(M_1(G))^2 + ID(G) - \frac{s^2}{2t}$. Equality holds if and only if G is regular.

3. Conclusion: In this article, we have presented several upper and lower bounds for RZ-invariant for a connected graph.

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