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Bounds for the First Zagreb Eccentricity Index and First Zagreb Degree Eccentricity Index

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Abstract. The first Zagreb eccentricity index $E_1(G)$ of a graph G is defined as the sum of squares of the eccentricities of the vertices. In this paper some bounds for the first Zagreb eccentricity index and first Zagreb degree eccentricity index are computed. –

1. Introduction

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. According to the IUPAC definition,[15] a topological index (or molecular structure descriptor) is a numerical value associated with chemical constitution for correlation of chemical structure with various physical properties, chemical reactivity or biological activity.

All the graphs $G = (V, E)$ considered in this paper are simple, undirected and connected graphs. The number of vertices of G is denoted by n and the number of edges is denoted by m, thus $|V(G)| = n$ and $|E(G)| = m$. For any vertices $u, v \in V(G)$, the distance $d(u, v)$ is defined as the length of any shortest path connecting u and v in G. For any vertex v_i in G, the degree (d_i or $d(v_i)$) of v_i is the number of edges incident with v_i in G. Especially, $\Delta = \Delta(G)$ and $\delta = \delta(G)$ are called the maximum and minimum degree of G, respectively. The eccentricity (e_i or $e(v_i)$) of v_i is the largest distance between v_i and any other vertex of G. The radius $r = r(G)$ is the minimum eccentricity among the vertices of G. The

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diameter $d = d(G)$ is the maximum eccentricity among the vertices of G. Also the second maximum eccentricity is written as d_2. A graph G is equi-eccentric if the eccentricity of every vertex is same [9].

The Zagreb indices were introduced by Gutman and Trinajstić in 1972 [8]. The main properties of $M_1(G)$ and $M_2(G)$ were summarized in [12]. The first Zagreb index $M_1(G)$ of G is defined as $M_1(G) = \sum\limits_{v_i \in V(G)} d_i^2$. The second Zagreb index $M_2(G)$ of G is defined as $M_2(G) = \sum\limits_{v_i v_j \in E(G)} d_i d_j$.

The invariants based on vertex eccentricities attracted some attention in Chemistry. In an analogy with the first and the second Zagreb indices, M. Ghorbani et al. and D. Vukičević et al. introduced the Zagreb eccentricity indices [7, 14]. The first Zagreb eccentricity index (E_1) of a graph G is defined as $E_1(G) = \sum\limits_{v_i \in V(G)} e_i^2$.

The Zagreb degree eccentricity indices are introduced in [13]. First Zagreb degree eccentricity index (DE_1) of a graph G is defined as $DE_1 = \sum\limits_{v_i \in V(G)} (e_i + d_i)^2$.

The total eccentricity index of G is defined as $\zeta(G) = \sum\limits_{v_i \in V(G)} e_i$. Fathalikhani et al. [6] have studied total eccentricity of some graph operations. Nilanjan De et al. [4] have studied total eccentricity index of the Generalized Hierarchical Product of Graphs.

In this paper we obtain some bounds for the first Zagreb eccentricity index and first Zagreb degree eccentricity index.

2. Main Results

Theorem 2.1.([1]) *Suppose a_i and b_i $1 \le i \le n$ are positive real numbers, then*

$$\left| n \sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \le \alpha(n)(A - b)(B - b) \tag{2.1}$$

where a, b, A and B are real constants, that for each i, $1 \le i \le n$, $a \le a_i \le A$ and $b \le b_i \le B$. Further, $\alpha(n) = n\lceil \frac{n}{2} \rceil (1 - \frac{1}{n} \lceil \frac{n}{2} \rceil)$, where $\lceil x \rceil$ largest integer greater than or equal to x.

We can see the appearance of Theorem 2.1, in [10].

Theorem 2.2. *Let G be a nontrivial graph of order n, then*

$$E_1(G) \le \frac{\alpha(n)(d - r)^2 + [\zeta(G)]^2}{n}.$$

Further, equality holds if and only if G is a equi-eccentric graph.

Proof. Let $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ be real numbers for which there exist real constants a, b, A and B, so that for each i, $i = 1, 2, \dots, n$, $a \leq a_i \leq A$ and $b \leq b_i \leq B$. Then by Theorem 2.1, the following inequality is valid

$$\left| n \sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \leq \alpha(n)(A-b)(B-b) \tag{2.2}$$

where $\alpha(n) = n\lceil \frac{n}{2} \rceil (1 - \frac{1}{n} \lceil \frac{n}{2} \rceil)$. Equality holds if and only if $a_1 = a_2 = \cdots = a_n$ and $b_1 = b_2 = \cdots = b_n$.
We choose $a_i = e_i = b_i$, $A = d = B$ and $a = r = b$, inequality (2.2) becomes

$$n \sum_{i=1}^{n} e_i^2 - \left(\sum_{i=1}^{n} e_i \right)^2 \leq \alpha(n)(d-r)(d-r)$$

$$nE_1(G) \leq \alpha(n)(d-r)^2 + [\zeta(G)]^2$$

$$E_1(G) \leq \frac{\alpha(n)(d-r)^2 + [\zeta(G)]^2}{n}.$$

Since equality in (2.2) holds if and only if $a_1 = a_2 = \cdots = a_n$ and $b_1 = b_2 = \cdots = b_n$, it follows that for each vertex of a graph G has same eccentricity, equality of the theorem holds if and only if equi-eccentric graph. □

Corollary 2.3. $E_1(G) \leq \dfrac{n^2(d-r)^2 + 4[\zeta(G)]^2}{4n}$.

Proof. Since $\alpha(n) \leq \dfrac{n^2}{4}$, the proof follows by above theorem. □

Theorem 2.4. *Let G be a nontrivial graph of order n, then*

$$E_1(G) \leq (r+d)\zeta(G) - rdn.$$

Equality holds if and only if G is equi-eccentric graph.

Proof. Let $a_1, a_2, \dots, a_n$ and $b_1, b_2, \dots, b_n$ be real numbers for which there exist real constants t and T, such that, $ta_i \leq b_i \leq Ta_i$ for each i, $1 \leq i \leq n$. Then the following inequality is valid (see [5])

$$\sum_{i=1}^{n} b_i^2 + tT \sum_{i=1}^{n} a_i^2 \leq (t+T) \sum_{i=1}^{n} a_i b_i \tag{2.3}$$

Equality of (2.3) holds if and only if $ta_i = b_i = Ta_i$ for at least one i, $1 \leq i \leq n$
We choose $b_i = e_i$, $a_i = 1$, $t = r$ and $T = d$ in inequality (2.3) then

$$\sum_{i=1}^{n} e_i^2 + rd \sum_{i=1}^{n} 1 \leq (r+d) \sum_{i=1}^{n} e_i$$

$$E_1(G) + rdn \leq (r+d)\zeta(G)$$

$$E_1(G) \leq (r+d)\zeta(G) - rdn.$$

If $ta_i = b_i = Ta_i$ for some i, then $b_i = t = T$. Therefore equality holds if and only if $r = d$, that is G is a equi-eccentric graph. $\square$

Theorem 2.5. *Let G be a nontrivial graph of order n and size m, then*

$$DE_1(G) \leq \frac{\alpha(n)(d+\Delta-r-\delta)^2 + [\zeta(G)+2m]^2}{n}.$$

Proof. Let $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ be real numbers for which there exist real constants a, b, A and B, so that for each i, $i = 1, 2, \ldots, n$, $a \leq a_i \leq A$ and $b \leq b_i \leq B$. Then by Theorem 2.1, the following inequality is valid

$$\left| n\sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \leq \alpha(n)(A-b)(B-b) \tag{2.4}$$

Equality holds if and only if $a_1 = a_2 = \cdots = a_n$ and $b_1 = b_2 = \cdots = b_n$.
We choose $a_i = e_i + d_i = b_i$, $A = d + \Delta = B$ and $a = r + \delta = b$, inequality (2.4) becomes

$$\begin{aligned} n\sum_{i=1}^{n}(e_i+d_i)^2 - \left[\sum_{i=1}^{n}(e_i+d_i)\right]^2 &\leq \alpha(n)(d+\Delta-r-\delta)(d+\Delta-r-\delta) \\ nDE_1(G) &\leq \alpha(n)(d+\Delta-r-\delta)^2 + \left[\sum_{i=1}^{n} e_i + \sum_{i=1}^{n} d_i\right]^2 \\ nDE_1(G) &\leq \alpha(n)(d+\Delta-r-\delta)^2 + [\zeta(G)+2m]^2 \\ DE_1(G) &\leq \frac{\alpha(n)(d+\Delta-r-\delta)^2 + [\zeta(G)+2m]^2}{n}. \end{aligned}$$

Since equality in 2.4 holds if and only if $a_1 = a_2 = \cdots = a_n$ and $b_1 = b_2 = \cdots = b_n$, the equality of the theorem holds if and only if $e_i + d_i$ is same for all the vertices of G. $\square$

Corollary 2.6. $DE_1(G) \leq \dfrac{n^2(d+\Delta-r-\delta)^2 + 4[\zeta(G)+2m]^2}{4n}$.

Proof. Since $\alpha(n) \leq \frac{n^2}{4}$, the proof follows by above theorem. $\square$

Theorem 2.7. *Let G be a nontrivial graph of order n and size m, then*

$$DE_1(G) \leq (d+\Delta+r+\delta)[\zeta(G)+2m] - (r+\delta)(d+\Delta)n.$$

Proof. Let $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ be real numbers for which there exist real constants t and T, so that for each i, $i = 1, 2, \ldots, n$, $ta_i \leq b_i \leq Ta_i$. Then the following inequality is valid (see [5])

$$\sum_{i=1}^{n} b_i^2 + tT\sum_{i=1}^{n} a_i^2 \leq (t+T)\sum_{i=1}^{n} a_i b_i \tag{2.5}$$

Equality of (2.5) holds if and only if, $ta_i = b_i = Ta_i$ for at least one i, $1 \leq i \leq n$
We choose $b_i = e_i + d_i$, $a_i = 1$, $t = r + \delta$ and $T = d + \Delta$ in inequality (2.5), then

$$\sum_{i=1}^{n}(e_i + d_i)^2 + (r+\delta)(d+\Delta)\sum_{i=1}^{n} 1 \leq (r+\delta+d+\Delta)\sum_{i=1}^{n}(e_i+d_i)$$

$$DE_1(G) + (r+\delta)(d+\Delta)n \leq (r+\delta+d+\Delta)[\zeta(G)+2m]$$

$$DE_1(G) \leq (r+\delta+d+\Delta)[\zeta(G)+2m] - (r+\delta)(d+\Delta)n.$$

If $ta_i = b_i = Ta_i$ for some i, then $t = b_i = T$. Therefore equality holds if and only if $r + \delta = e_i + d_i = d + \Delta$ for some i. i.e., $r = e_i = d$ and $\delta = d_i = \Delta$ for some i. Therefore equality of the theorem holds if and only if $e_i + d_i$ is same for all the vertices of G. □

Lemma 2.8.([2]) *For positive real numbers* $a_1, a_2, \ldots, a_k$

$$A^{\frac{1}{2}} \geq B^{\frac{1}{(k-1)}},$$

where

$$A = \frac{2}{k(k-1)}(a_1a_2 + a_1a_3 + \cdots + a_1a_n + a_2a_3 + \cdots + a_{k-1}a_k),$$

$$B = \frac{1}{k}(a_1a_2\cdots a_{k-1} + a_1a_2\cdots a_{k-2}a_k + \cdots + a_2a_3\cdots a_{k-1}a_k).$$

Equality holds if and only if $a_1 = a_2 = \cdots = a_k$.

The Lagrange identity is as follows.

Lemma 2.9.([11]) *Let* $(a) = (a_1, a_2, \ldots, a_k)$, $(b) = (b_1, b_2, \ldots, b_k)$ *be two real* $k-$*tuples. Then*

$$\sum_{i=1}^{k} a_i^2 \sum_{j=1}^{k} b_j^2 - \left(\sum_{i=1}^{k} a_i b_i\right)^2 = \sum_{1\leq i<j\leq k}(a_ib_j - a_jb_i)^2.$$

Theorem 2.10. *Let* G *be a nontrivial graph of order* n *and size* m, *then*

(2.6)
(i) $E_1(G) \geq d^2 + \dfrac{[\zeta(G)-d]^2}{(n-1)} + \dfrac{2(n-2)}{(n-1)^2}(d_2 - r)^2$

with equality if and only if G *is a star,*

(2.7)
(ii) $E_1(G) \leq 2d^2 + \zeta^2(G) - 2d\zeta(G) - (n-1)(n-2)\left[\dfrac{1}{(n-1)d}\prod_{j=1}^{n} e_j \left[\left(\sum_{i=1}^{n}\dfrac{1}{e_i}\right) - \dfrac{1}{d}\right]\right]$

with equality if and only if G is a star.

Proof. (i) If we set $k = n-1$, $a_i = e_{i+1}$, $b_i = 1$, $i = 1, 2, \ldots, k$ in Lemma 2.9 then we get

$$(n-1)\sum_{i=2}^{n} e_i^2 - \left(\sum_{i=2}^{n} e_i\right)^2 = \sum_{2\le i<j\le n} (e_i - e_j)^2$$

If $e_i \ge e_j$, $i \le j$ then $e_1 = d$ and hence

$$(n-1)[E_1(G) - d^2] = [\zeta(G) - d]^2 + \sum_{2\le i<j\le n} (e_i - e_j)^2 \tag{2.8}$$

Now,

$$\begin{aligned}\sum_{2\le i<j\le n} [e_i - e_j] &= (n-2)e_2 - \sum_{i=3}^{n} e_i + \sum_{3\le i<j\le n-1} [e_i - e_j] + \sum_{i=3}^{n-1} e_i - (n-3)e_n \\ &= (n-2)(e_2 - e_n) + \sum_{3\le i<j\le n-1} [e_i - e_j] \\ &\ge (n-2)(d_2 - r). \qquad (2.9)\end{aligned}$$

By power-mean inequality [3], we have

$$\left(\frac{\sum\limits_{2\le i<j\le n} (e_i - e_j)^2}{\frac{(n-1)(n-2)}{2}}\right)^{\frac{1}{2}} \ge \frac{\sum\limits_{2\le i<j\le n} [e_i - e_j]}{\frac{(n-1)(n-2)}{2}}$$

with equality if and only if

$$(e_i - e_j) = (e_l - e_m)$$

for any $2 \le i, j, l, m \le n$, that is $e_2 = e_3 = \cdots = e_{n-1} = e_n$.
From the above, we get

$$\sum_{2\le i<j\le n} (e_i - e_j)^2 \ge \frac{2}{(n-1)(n-2)} \left(\sum_{2\le i<j\le n} [e_i - e_j]\right)^2 \tag{2.10}$$

with equality if and only if $e_2 = e_3 = \cdots = e_{n-1} = e_n$.
Using (2.9), from the above, we get

$$\sum_{2\le i<j\le n} (e_i - e_j)^2 \ge \frac{2(n-2)}{(n-1)} (d_2 - r)^2$$

Using the above result in (2.8), we get (2.6). First part of proof is done. Now, suppose that the equality holds in (2.6). Then the equality holds in (2.9) and (2.10). From the equality in (2.9), we get $e_3 = \cdots = e_{n-1}$. From the equality in (2.10), we get $e_2 = e_3 = \cdots = e_{n-1} = e_n$. Hence G is a star graph.

Conversely, suppose $e_2 = e_3 = \cdots = e_{n-1} = e_n = r$. Then we have

$$\zeta(G) = d + (n-1)r$$

that is,

$$r = \frac{\zeta(G) - d}{(n-1)}$$

Using the above result we get

$$\begin{aligned} E_1(G) &= d^2 + (n-1)r^2 \\ &= d^2 + \frac{[\zeta(G) - d]^2}{(n-1)} \\ &= d^2 + \frac{[\zeta(G) - d]^2}{(n-1)} + \frac{2(n-2)}{(n-1)^2}(d_2 - r)^2 \quad as \quad d_2 = r \end{aligned}$$

(ii) If we set $k = n-1$, $a_i = e_{i+1}$, $i = 1, 2, \ldots, k$ in Lemma 2.8, then we get

$$\begin{aligned} \sum_{2 \le i < j \le n} e_i e_j &\ge \frac{(n-1)(n-2)}{2} \left[\frac{1}{n-1} \prod_{j=2}^{n} e_j \sum_{i=2}^{n} \frac{1}{e_i} \right]^{\frac{2}{n-2}} \\ &= \frac{(n-1)(n-2)}{2} \left[\frac{1}{(n-1)d} \prod_{j=1}^{n} e_j \left[\left(\sum_{i=1}^{n} \frac{1}{e_i} \right) - \frac{1}{d} \right] \right]^{\frac{2}{n-2}} \end{aligned} \tag{2.11}$$

But,

$$\begin{aligned} &\sum_{2 \le i < j \le n} (e_i - e_j)^2 \\ &= (n-2) \sum_{i=2}^{n} e_i^2 - 2 \sum_{2 \le i < j \le n} e_i e_j \\ &\le (n-2)[E_1(G) - d^2] - (n-1)(n-2) \left[\frac{1}{(n-1)d} \prod_{j=1}^{n} e_j \left[\left(\sum_{i=1}^{n} \frac{1}{e_i} \right) - \frac{1}{d} \right] \right]^{\frac{2}{n-2}} \end{aligned}$$

using the above result in (2.8), we get the upper bound in (2.7). First part of the proof is done.

The equality holds in (2.7) if and only if the equality holds in (2.11), that is, $e_2 = e_3 = \cdots = e_{n-1} = e_n$, by Lemma 2.8. Hence, the equality holds in (2.7) if and only if G is a star graph. □

Conclusion

In this paper we have established some bounds of the first Zagreb eccentricity index and first Zagreb degree eccentricity index in terms of some graph parameters such as order, size, maximum and minimum degree, radius, diameter and total eccentricity index. It may be useful to give the bounds for $E_1(G)$, $E_2(G)$, $DE_1(G)$ and $DE_2(G)$ indices in terms of other graph invariants.

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