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Some topological indices of graphs and some inequalities

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ABSTRACT

Let G be a graph. In this paper, we study the eccentric connectivity index, the new version of the second Zagreb index and the forth geometric–arithmetic index.. The basic properties of these novel graph descriptors and some inequalities for them are established.

Keywords: Topological index, eccentric connectivity, geometric–arithmetic, Zagreb index, Cauchy–Schwarz inequality.

1. INTRODUCTION

A topological index for a graph is a numerical quantity which is invariant under automorphisms of the graph. The simplest topological indices are the number of vertices and edges of the graph. Throughout this paper, all graphs are assumed to be simple connected with $n > 1$ vertices and m edges that are undirected.

In the last few years, the number of proposed molecular descriptors is rapidly growing [1]. A special class of these descriptors comprises is called topological indices. Topological indices are usually defined via the molecular graph. Graph theory is a mathematical discipline belonging to discrete mathematics. For more information on graph theory and application in chemistry we refer to [2−5]. Suppose that $G = (V, E)$ is a graph with the vertex set V and the edge set E, that $|V| = n$ and $|E| = m$. One of the recent molecular descriptors defined by graph degree is the geometric–arithmetic indices of graphs and its variants. The general formula for the geometric–arithmetic index is given by $GA_{general}(G) = \sum_{uv\in E}(2\sqrt{Q_u Q_v})/(Q_u + Q_v)$, where for a vertex x, the number Q_u is

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some quantity that, in a unique manner, can be associated with the vertex u [6–14]. As yet, for topological indices belonging to the GA-family have been conceived, named as the first GA_1, second GA_2, third GA_3 and the fourth geometric–arithmetic index GA_4. The first geometric–arithmetic index of a graph G is defined as $GA_1(G) = \sum_{uv\in E}(2\sqrt{d_u d_v})/(d_u + d_v)$, where d_x is the degree of the vertex x in the graph G. The second geometric–arithmetic index is calculated by the formula $GA_2(G) = \sum_{uv\in E} 2\sqrt{n_u n_v}/(n_u + n_v)$, where for any edge $e = uv$, n_u is the number of vertices that are closer to the vertex u than to the vertex v and n_v is defined analogously. The third geometric–arithmetic index is defined by the formula $GA_3(G) = \sum_{uv\in E} 2\sqrt{m_u m_v}/(m_u + m_v)$, where for any edge $e = uv$, m_u is the number of edges that are closer to the vertex u than to the vertex v and m_v is defined analogously.

Let a, b, x be vertices and $e = uv$ be an edge of a graph G. The distance between a and b that denoted by $d(a,b)$ is the length of a shortest path connecting a and b in the graph G. The distance between the vertex x and the edge $e = uv$ is defined by $d(x,\ uv) = \min\{d(x,u), d(x,v)\}$. The eccentricity of a vertex x is denoted by ε_x and is given by $\varepsilon_x = Max\{d(x,y) \mid y \in V\}$. The maximum value of eccentricity over all vertices of G is called the diameter of G and denoted by $D(G)$. Also, the minimum value of eccentricity among the vertices of G is called the radius of G and denoted by $r(G)$. The eccentric connectivity index $\xi(G)$ of the graph G is defined as $\xi(G) = \sum_{x\in V} d_x\varepsilon_x = \sum_{e=uv\in E}(\varepsilon_u + \varepsilon_v)$. The fourth geometric–arithmetic index GA_4 of G is defined as $GA_4(G) = \sum_{e=uv\in E} 2\sqrt{\varepsilon_u\varepsilon_v}/(\varepsilon_u + \varepsilon_v)$.

The Zagreb group indices of a graph G have been introduced more than thirty years ago by Gutman and Trinajstic [15]. Ghorbani [16] has defined two new version of Zagreb indices as follows: $M_1^*(G) = \sum_{e=uv\in E}[\varepsilon_u + \varepsilon_v]$ and $M_2^*(G) = \sum_{e=uv\in E} \varepsilon_u\varepsilon_v$. It is easy to see that for any graph G, $M_1^*(G) = \xi(G)$.

2. EXAMPLES

Directly from the definition, we calculate the eccentric connectivity, the fourth geometric–arithmetic and the new second Zagreb indices of the n–vertex complete graph K_n, the complete bipartite graph $K_{r,t}$, the n–vertex cycle graph C_n, the n–vertex path P_n and the $(n+1)$–vertex star S_n. These are as follows:

$\xi(K_n) = 2m = n(n-1)$, $GA_4(K_n) = m = \frac{n(n-1)}{2}$, $M_2^*(K_n) = m = \frac{n(n-1)}{2}$, $\xi(K_{r,t}) = 4m = 4rt$, $GA_4(K_{r,t}) = m = rt$ and $M_2^*(K_n) = m = \frac{n(n-1)}{2}$. If n is even, then for $x \in V, \varepsilon_x = \frac{n}{2}$ and $\xi(C_n) = n^2$, $GA_4(C_n) = n$, $M_2^*(C_n) = \frac{n^3}{4}$. If n is odd, then for all $x \in V, \varepsilon_X = \frac{n-1}{2}$, $\xi(C_n) = n(n-1)$ and $GA_4(C_n) = n$ $M_2^*(C_n) = \frac{n(n-1)^2}{4}$.

If n is even, then $\xi(P_n) = \frac{n(3n-2)}{2}$, $GA_4(P_n) = 1 + 4\sum_{i=1}^{n/2}\frac{\sqrt{(n-i)(n-i-1)}}{2(n-i)-1}$ and $M_2^*(P_n) = \frac{n^2}{4} + 2\sum_{i=1}^{n/2}(n-i)(n-i-1)$. If n is odd then $\xi(P_n) = \frac{(n+1)(3n-5)}{2}$, $GA_4(P_n) = 4\sum_{i=1}^{(n+1)/2}\frac{\sqrt{(n-i)(n-i-1)}}{2(n-i)-1}$ and $M_2^*(P_n) = 2\sum_{i=1}^{(n+1)/2}(n-i)(n-i-1)$. Finally, $\xi(S_n) = 3n$, $GA_4(S_n) = \frac{2\sqrt{2}}{3}n$ and $M_2^*(S_n) = 2n$.

In this paper, the main properties of ξ, GA_4 and M_2^* indices of graphs are established and some bounds for these indices with relation between them are presented.

3. MAIN RESULTS AND DISCUSSION

In this section, at first we calculate some bounds for the fourth geometric–arithmetic, the eccentric connectivity and new Zagreb indices of a graph, then present some relations between these indices. The famous inequality $\sqrt{ab} \le (a+b)/2 \le ab$ for any positive real numbers a,b with equality if and only if $a=b$ and also the Cauchy-Schwarz inequality have been used in the proof of the following propositions. Note that $G \cong K_n$ if and only if for all $e = uv \in E, \varepsilon_U = \varepsilon_V = 1$.

Proposition 1. For any graph G,

i) $\xi(G) \ge 2m$ with equality if and only if $G \cong K_n$,

ii) $GA_4(G) \le m$ with equality if and only if $\forall e = uv \in E, \varepsilon_u = \varepsilon_v = k$ for some k,

iii) $M_2^*(G) \ge m$ with equality if and only if $G \cong K_n$.

Proof. For proving this proposition, it is enough to notice that for all $\forall x \in V, \varepsilon_X \ge 1$, when $n > 1$. ■

Proposition 2. Suppose G is a graph with m edges. Then $GA_4(G) \geq 2m\sqrt{2}/3$ with equality if and only if $G \cong S_n$, where S_n denotes the $(n+1)-$ vertices star.

Proof. Since for any edges $e = uv$, $\varepsilon_u = \varepsilon_v$ or $|\varepsilon_u - \varepsilon_v| = 1$, we can assume that $\varepsilon_u \geq \varepsilon_v$. If $x = \varepsilon_v / \varepsilon_u$, then $2\sqrt{\varepsilon_u \varepsilon_v}/(\varepsilon_u + \varepsilon_v) = 2\sqrt{x}/(x+1)$. Suppose $f(x) = 2\sqrt{x}/(x+1)$. By derivation, we can conclude that f is increasing on the closed interval [1/2,1]. So, for any $x \in [1/2,1]$, $f(x) \geq f(1/2)$. This shows that $2\sqrt{x}/x+1 \geq 2\sqrt{2}/3$ and $GA_4(G) \geq 2m\sqrt{2}/3$. Now we prove that $GA_4(G) = 2m\sqrt{2}/3$ if and only if $G \cong S_n$. If $G \cong S_n$ then for any edge $e = uv$, $\varepsilon_u = 2$ and $\varepsilon_v = 1$, so $GA_4(G) = 2m\sqrt{2}/3$. If $GA_4(G) = 2m\sqrt{2}/3$ and G is not isomorphic to S_n, then there exists an edge $e = uv$ such that $\varepsilon_u \neq 2$ or $\varepsilon_v \neq 1$. Since $\varepsilon_u \geq 3$ or $\varepsilon_v \geq 2$, then for $x = \varepsilon_v / \varepsilon_u$, $2/3 \leq x \leq 1$ and so $2\sqrt{x}/(x+1) \geq 2\sqrt{6}/5$. In this case, $GA_4(G) \geq 2\sqrt{2}(m-1)/3 + 2\sqrt{6}/5 > 2m\sqrt{2}/3$. ■

Note. It is easy to see that if $E' \subseteq E$ with $|E'| = m'$ then $2m'\sqrt{2}/3 \leq \sum_{e=uv\in E} \frac{2\sqrt{\varepsilon_u \varepsilon_v}}{\varepsilon_u + \varepsilon_v} \leq m'$.

In this part, we present some relationships between the fourth geometric–arithmetic index $GA_4(G)$, the Eccentric connectivity index $\xi(G)$ and new Zagreb index $M_2^*(G)$ of a graph G.

Proposition 3. Suppose G is a graph then $GA_4(G) \geq 2m/n$.

Proof. Since for any vertex x, $1 \leq \varepsilon_x \leq n-1$ where $n > 1$, we can conclude that

$$\frac{2\sqrt{\varepsilon_u \varepsilon_v}}{\varepsilon_u + \varepsilon_v} \geq \frac{2\sqrt{\varepsilon_u}}{\varepsilon_u + (n-1)}.$$

If $f(x) = 2\sqrt{x}/(x + (n-1))$, then one can see the function f is increasing on the closed interval $[1, n-1]$. Therefore, for all $x \in V$, $\frac{2\sqrt{\varepsilon_x}}{\varepsilon_x + (n-1)} \geq f(1) = \frac{2}{n}$ and so $GA_4(G) \geq \frac{2m}{n}$. ■

Proposition 4. $GA_4 \leq 1/2\xi(G) \leq M_2^*(G)$ with equality if and only if $G \cong K_n$.

Proof. Since $\varepsilon_x \geq 1$ for any vertex *x*, we can conclude that for any edge $e = uv, \varepsilon_u + \varepsilon_v \geq 2$.

Therefore, we have: $\frac{2\sqrt{\varepsilon_u \varepsilon_v}}{\varepsilon_u + \varepsilon_v} \leq 1 \leq \frac{\varepsilon_u + \varepsilon_v}{2} \leq \varepsilon_u \varepsilon_v$ and then $GA_4 \leq \frac{1}{2}\xi(G) \leq M_2^*(G)$ with equality if and only if for any edge $e = uv$ we have $\varepsilon_u = \varepsilon_v = 1$, which completes our proof. ■

Proposition 5. Let G be a graph then $GA_4(G) \leq \sqrt{mM_2^*(G)}$ with equality if and only if $G \cong K_n$.

Proof. Since $\forall e = uv, \frac{2\sqrt{\varepsilon_u \varepsilon_v}}{\varepsilon_u + \varepsilon_v} \leq \sqrt{\varepsilon_u \varepsilon_v}$ and by applying the Cauchy–Schwarz Inequality, $\sum_{e=uv} \sqrt{\varepsilon_u \varepsilon_v} = \sum_{e=uv} 1.\sqrt{\varepsilon_u \varepsilon_v} \leq \sqrt{\sum_{e=uv} 1 \sum_{e=uv} \varepsilon_u \varepsilon_v} = \sqrt{mM_2^*(G)}$. Therefore $GA_4(G) \leq \sqrt{mM_2^*(G)}$ with equality if and only $\varepsilon_u = \varepsilon_v = 1$. Thus $G \cong K_n$. If $G \cong K_n$ then $GA_4(G) = M_2^*(G) = m$, $\sqrt{mM_2^*(G)} = m$ and so $GA_4(G) = \sqrt{mM_2^*(G)}$. ■

Proposition 6. Let G be a graph then $GA_4(G) \leq \sqrt{M_2^*(G) + m(m-1)}$ with equality if and only if $G \cong K_n$.

Proof. By applying the hypothesis in the proof of Proposition 4, we can see $GA_4(G)^2 \leq \sum_{e=uv \in E_1} \varepsilon_u \varepsilon_v + \sum_{\substack{e=uv \in E \\ e'=xy \\ e \neq e'_1}} \frac{2\sqrt{\varepsilon_u \varepsilon_v}}{\varepsilon_u + \varepsilon_v} \frac{2\sqrt{\varepsilon_x \varepsilon_y}}{\varepsilon_x + \varepsilon_y} \leq M_2^*(G) + m(m-1)$. Therefore, $GA_4(G) \leq \sqrt{M_2^*(G) + m(m-1)}$. Now we claim that equality holds if and only if $GA_4(G) = M_2^*(G) = m$ if and only if $\forall e = uv \in E, \varepsilon_u = \varepsilon_v = 1$ if and only if $G \cong K_n$. ■

Note. we can see that if for an edge $e = uv, \varepsilon_u = n-1$, then $\varepsilon_v = n-2$. Therefore, for each $e = uv$, $2 \leq \varepsilon_u + \varepsilon_v \leq 2n-3$.

Proposition 7. If G is a graph then $GA_4(G) \geq \frac{2}{2n-3}\sqrt{M_2^*(G) + m(m-1)}$.

Proof. By definition,

$$[GA_4(G)]^2 = \sum_{e=uv\in E}[\frac{2\sqrt{\varepsilon_u\varepsilon_v}}{\varepsilon_u+\varepsilon_v}]^2 + 2\sum_{uv\neq xy}[\frac{2\sqrt{\varepsilon_u\varepsilon_v}}{\varepsilon_u+\varepsilon_v}\frac{2\sqrt{\varepsilon_x\varepsilon_y}}{\varepsilon_x+\varepsilon_y}]$$

$$\geq \sum_{e=uv\in E}\frac{4\varepsilon_u\varepsilon_v}{(2n-3)^2} + 2\sum_{uv\neq xy}(\frac{2}{2n-3})^2$$

$$= \frac{4}{(2n-3)^2}[M_2^*(G)+m(m-1)],$$

and so $GA_4(G) \geq \frac{2}{2n-3}\sqrt{M_2^*(G)+m(m-1)}$. ■

Proposition 8. Let G be a graph, then $GA_4(G) \leq \left\lceil \frac{m-1}{2} \right\rceil + \sqrt{\left\lceil \frac{m-1}{2} \right\rceil^2 + M_2^*(G)}$ with equality if and only if $G \cong K_2$.

Proof. Take $\left\lceil \frac{m-1}{2} \right\rceil = t$, so

$$[GA_4(G)]^2 = \sum_{e=uv\in E}[\frac{2\sqrt{\varepsilon_u\varepsilon_v}}{\varepsilon_u+\varepsilon_v}]^2 + 2\sum_{uv\neq xy}[\frac{2\sqrt{\varepsilon_u\varepsilon_v}}{\varepsilon_u+\varepsilon_v}\frac{2\sqrt{\varepsilon_x\varepsilon_y}}{\varepsilon_x+\varepsilon_y}]$$

$$\leq \sum_{e=uv\in E}\varepsilon_u\varepsilon_v + 2tGA_4(G) = M_2^*(G) + 2tGA_4(G).$$

Therefore $[GA_4(G)-t]^2 \leq M_2^*(G)+t^2$ and so $GA_4(G) \leq \left\lceil \frac{m-1}{2} \right\rceil + \sqrt{\left\lceil \frac{m-1}{2} \right\rceil^2 + M_2^*(G)}$. The equality holds if and only if $G \cong K_2$. ■

Proposition 9. If G is a graph, then $\xi(G) > \frac{4}{2n-3}M_2^*(G)$.

Proof. Note that any positive real numbers a,b satisfy the inequality $(a+b)^2 \geq 4ab$ and equality holds if and only if $a=b=1$. We can easily to see that $(2n-3)\xi(G) \geq \sum_{e=uv\in E}(\varepsilon_u+\varepsilon_v)^2 \geq \sum_{e=uv\in E}4\varepsilon_u\varepsilon_v = 4M_2^*(G)$, so $\xi(G) \geq \frac{4}{2n-3}M_2^*(G)$ with equality if and only if $\forall e=uv\in E, \varepsilon_u=\varepsilon_v=1$ if and only if $\xi(G)=n(n-1)$ and $\frac{4}{2n-3}M_2^*(G) = \frac{2n(n-1)}{2n-3}$ if and only if $2n=5$ that is a contradiction. So $\xi(G) > \frac{4}{2n-3}M_2^*(G)$. ■

Proposition 10. Suppose that G is a graph, then the following statements hold:
i) $\xi(G)^2 \geq 4M_2^*(G)$,
ii) $\xi(G)^2 \geq [2m + 2M_2^*(G)]$,
iii) $\xi(G)^2 \geq [\xi(G) + 2M_2^*(G)]$.

Proof. The proof of this proposition by applying the inequality $\frac{a+b}{2} \leq ab$ for any positive real numbers a, b is similar to the proof of propositin9 and it is omitted. ■

Proposition 11. Let G is a graph.
i) If $\forall e = uv \in E, \min\{\varepsilon_u, \varepsilon_v\} = 1$, then $\xi(G) > M_2^*(G)$;
ii) If $\forall e = uv \in E, \min\{\varepsilon_u, \varepsilon_v\} > 1$, then $\xi(G) < M_2^*(G)$.

Proof. To prove this proposition, it is enough to notice that if $\forall e = uv \in E, \min\{\varepsilon_u, \varepsilon_v\} = 1$, then $\varepsilon_u + \varepsilon_v > \varepsilon_u \varepsilon_v$ and if $\forall e = uv \in E, \min\{\varepsilon_u, \varepsilon_v\} > 1$, then $\varepsilon_u + \varepsilon_v < \varepsilon_u \varepsilon_v$. ■

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REFERENCES

1. R. Todeschini and V. Consonni, Molecular Descriptors for Chemoinformatics, Wiley–VCH, *Weinheim*, 2009.
2. H. Hosoya, Topological index, A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, *Bull. Chem. Soc. Japan.,* **44** (1971) 2332−2339.
3. A. Graovac, O. Ori, M. Faghani and A. R. Ashrafi, Distance Property of Fullerenes, *Iranian J. Math. Chem.,* **2** (1) (2011) 99−107.
4. G. H. Fath–Tabar, M. J. Nadjafi–Arani, M. Mogharrab and A. R. Ashrafi, Some Inequalities for Szeged–Like Topological Indices of Graphs, *MATCH Commun. Math. Comput. Chem.,* **63** (2010) 145−150.
5. Z. Yarahmadi and S. Moradi, Second and third extremals of catacondensed hexagonal systems with respect to the PI index, *Iranian J. Math. Chem.,* **1** (1) (2010) 95−103.
6. D. Vukičević and 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.

7. B. Zhou, I. Gutman, B. Furtula and Z. Du, On two types of geometric−arithmetic index, *Chem. Phys. Lett.,* **482** (2009) 153−155.
8. K. C. Das, On geometric−arithmetic index of graphs, *MATCH Commun. Math. Comput. Chem.,* **64** (2010) 619−630.
9. Y. Yuan, B. Zhou and N. Trinajstić, On geometric−arithmetic index, *J. Math. Chem.,* **47** (2010) 833−841.
10. M. Mogharrab and G. H. Fath–Tabar, Some bounds on GA_1 index of graphs, *MATCH Commun. Math. Comput. Chem.,* **65** (2011) 33−38.
11. G. H. Fath–Tabar, B. Furtula and I. Gutman, A new geometric–arithmetic index, *J Math Chem*., **47** (2010) 477–486.
12. G. H. Fath–Tabar, Old and new Zagreb indices of graphs, *MATCH Commun. Math. Comput. Chem.,* **63** (2011) 79−84.
13. G. H. Fath–Tabar, A. Hamzeh and S. Hossein-Zadeh, GA_2 index of some graph oprations, *FILOMAT*, **24(1)** (2010) 21−28.
14. G. H. Fath−Tabar, A. Azad and L. Elahinejad, Some Topological Indices of Tetrameric 1,3-Adamantane, *Iranian J. Math. Chem.,* **1(2)** (2010) 111−118.
15. I. Gutman and N. Trinajstić, Graph theory and molecular orbitals, Total π−electron energy of alternant hydrocarbons, *Chem. Phys. Lett.,* **17** (1972) 535−538.
16. M. Ghorbani, Personal communication, 2012.