On the Edge Version of Zagreb Coindex

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Abstract:-The first Zagreb coindex is the sum of degrees of non adjacent vertices of a graph G. In this paper the edge version of the first Zagreb coindex is defined as the reformulated Zagreb coindex. We explore here their basic mathematical properties and using these results, the reformulated Zagreb coindices of some classes of chemical graphs are computed.

Keywords:*Edge degree; reformulated Zagreb indices; reformulated Zagreb coindices.*
AMS Subject Classification: 05C90; 05C12.

1. Introduction

Let $G = (V, E)$ be a graph. The number of vertices of G we denote by $n$and the number of edges we denote by m, thus $|V(G)| = n$and $|E(G)| = m$. The degree of a vertex v, denoted by $d_G(v)$. Specially, $\Delta = \Delta(G)$ and $\delta = \delta(G)$ are called the maximum and minimum degree of vertices of G respectively. $G$is said to be r-regular if $\delta(G) = \Delta(G) = r$ for some positive integer r. The complement of a graph G, denoted by G, is a simple graph on the same set of vertices $V(G)$ in which two vertices u and v are connected by an edge uv, if and only if they are not adjacent in G .Obviously, $E(G) \cup E(\bar{G}) = E(K_n)$, and $\bar{m} = |E(\bar{G})| = \frac{n(n-1)}{2} - m$. The line graph $L(G)$ of a graph is the graph derived from G in such a way that the edges in G are replaced by vertices in $L(G)$ and two vertices in $L(G)$ are connected whenever the corresponding edges in G are adjacent [14]. The jump graph $J(G)$ of a graph G is the complement of a line graph [15].

The Zagreb indices were first introduced by Gutman and Trinajstić[12]. They are important molecular descriptors and have been closely correlated with many chemicalproperties[23,27,28]. There was a vast research concerning the mathematical properties and bounds for Zagreb indices and also their various variants [3–6,10,13,16–22,29–32].

$$M_1(G) = \sum_{u \in V(G)} d_G(u)^2 \qquad and \qquad M_2(G) = \sum_{uv \in E(G)} d_G(u)\, d_G(v).$$

In fact, one can rewrite the first Zagreb index as

$$M_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)].$$

Noticingthatcontributionofnonadjacentvertexpairsshouldbetakenintoaccount when computingtheweighted Wiener polynomials ofcertain compositegraphs(see [8]) definedfirstZagrebcoindexandsecondZagrebcoindexas

$$\overline{M_1}(G) = \sum_{uv \notin E(G)} [d_G(u) + d_G(v)] \qquad and \qquad \overline{M_2}(G) = \sum_{uv \notin E(G)} [d_G(u)\, d_G(v)].$$

For more information on Zagerbcoindices see [1,2].

Miličevićet. al [25] reformulatedtheZagrebindicesintermsofedge-degreesinstead of vertex-degrees:

$$EM_1(G) = \sum_{e \in E(G)} d_G(e)^2 \qquad and \qquad EM_2(G) = \sum_{e \sim f \in E(G)} d_G(e)\, d_G(f),$$

where$d_G(e)$ denotes the degree of an edge $e = uv$ in G, which is defined by $d_G(e) = d_G(u)+d_G(v) - 2$ and $e \sim f$means that the edges e and $f$are adjacent.The properties ofthereformulatedZagrebindicesarestudiedbyseveralresearchers[18,32].

Noticingthatcontributionofnonadjacentedgespairsshouldbetakenintoaccount, we define reformulated Zagreb coindices:

$$\overline{EM_1}(G) = \sum_{e \nsim f \notin E(G)} [d_G(e) + d_G(f)] \quad and \quad \overline{EM_2}(G) = \sum_{e \nsim f \notin E(G)} d_G(e)\, d_G(f).$$

where$d_G(e)$ denotes the degree of an edge $e = uv$ in $J(G)$, which is defined by $d_{J(G)}(e) = m + 1 - (d_G(u)+d_G(v))$ and $e \nsim f$means that the edges e and $f$are non adjacent.

2. Connection between original and reformulated Zagreb coindices

Because of the equalities that exist be between the complementofagraph$G$andjump graph$J(G)$,theoriginalandreformulatedZagrebcoindicesarerelatedasfollows:

$$\overline{EM_1}(G) = \overline{M_1}(J(G))$$

$$\overline{EM_2}(G) = \overline{M_2}(J(G))$$

The above relations can be easily verified.

Therefore, one can compute the edge-based Zagreb coindices of molecular graphs as the vertex based indices of corresponding jump graphs. Vertex-based Zagreb coindices appear to be easier to generate, because there is no ambiguities in assigning the vertex degrees. However, there is a price to paythe jump graph is almost always is a more complicated structure than the corresponding molecular graph, this can easily be confirmed by drawing a few simple graphs and the corresponding jump graphs. Thus, the user must decide whether it is simpler to construct the jump graph of a graph or to assign the edge-degrees to a graph.

3. MathematicalpropertiesoffirstreformulatedZa- grebcoindex

InthissectionwepresentupperandlowerboundsforthefirstreformulatedZagreb coindex.

Webeginwiththefollowingstraightforward,previouslyknown,auxiliaryresult.

Lemma1.[1]*LetGbeanynontrivialgraphofordernandsizem.Then*

$M_1(G) + \overline{M_1}(G) = 2m(n-1).$ (1)

Lemma 2.[9]*Let a_i and $b_i, i = 1,2,\dots,n$ be a real numbers such that $ma_i \le b_i \le Ma_i$for $i = 1,2,\dots,n$. Then*

$$\sum_{i=1}^{n} {b_i}^2 + mM \sum_{i=1}^{n} {a_i}^2 \le (M+m) \sum_{i=1}^{n} a_i b_i \qquad (2)$$

with equality if and only if either $b_i = ma_i$ or $b_i = Ma_i$ for every$i = 1,2,\dots,n$.

Lemma 3.[24]*Let $a_1 \ge a_2 \ge \cdots, \ge a_n$ and $b_1 \ge b_2 \ge \cdots, \ge b_n$ be a real numbers. Then*

$$n \sum_{i=1}^{n} a_i b_i \ge \sum_{i=1}^{n} a_i \cdot \sum_{i=1}^{n} b_i \qquad (3)$$

with equality if and only if$a_1 = a_2 = \cdots, = a_n$or $b_1 = b_2 = \cdots, = b_n$.

Proposition 1.*Let G be any nontrivial graph of order n and size m. Then*

$$\overline{EM_1}(G) = 2\overline{m}(m+1) - 4m(n-1) - 2M_1(G) \qquad (4)$$

where$\overline{m}$is the number of edges in $\overline{G}$.

Proof. It is easily seen that

$$\overline{EM_1}(G) = \sum_{uv \notin E(G)} (m+1-(d_G(u)+d_G(v))) + (m+1-(d_G(u)+d_G(v)))$$

$$= 2(m+1)\overline{m} - 2\overline{M_1}(G)$$

$$= 2\overline{m}(m+1) - 2[2m(n-1) - M_1(G)]$$

$$= 2\overline{m}(m+1) - 4m(n-1) + 2M_1(G)]$$

As asserted.

Theorem2.*Let G be any nontrivial graph of order n and size m. Then*

$$\overline{EM_1}(G) \leq 2\overline{m}(m+1) - 4m(\Delta+\delta+n-1) - 2n\delta\Delta. \quad (5)$$

Proof. By setting $b_i = d_G(v_i)$ and $a_i = 1$in Lemma 2, we have $\delta a_i \leq b_i \leq \Delta a_i$ and

$$\sum_{i=1}^{n} d_G(v_i)^2 + \delta\Delta \sum_{i=1}^{n} 1 \leq (\Delta+\delta)2m$$

$$M_1(G) \leq (\Delta+\delta)2m - \Delta\delta n.$$

By Proposition 1, it follows that

$$\overline{EM_1}(G) \leq 2\overline{m}(m+1) - 4m(\Delta+\delta+n-1) - 2n\delta\Delta$$

Theorem3.*Let G be any nontrivial graph of order n and size m. Then*

$$\overline{EM_1}(G) \geq 2\overline{m}(m+1) - 4m(n-1) + \frac{8m^2}{n} \quad (6)$$

with equality if and only if G is regular.

Proof. By setting $a_i = b_i = d_G(v_i)$ in Lemma 3, we have $M_1(G) \geq \frac{4m^2}{n}$

Therefore, by proposition 1, it follows that

$$\overline{EM_1}(G) \geq 2\overline{m}(m+1) - 4m(n-1) + \frac{8m^2}{n}$$

4. Mathematicalpropertiesofsecondreformulated Zagreb coindex

Proposition4.*LetGbeanynontrivialgraphofordernandsizem.Then*

$$\overline{EM_2}(G) = \overline{m}(m+1)^2 + \sum_{uv \notin E(G)} (d_G(u)^2 + d_G(v)^2) + 2\overline{M_2}(G) - 2(m+1)\overline{M_1}(G). \quad (7)$$

where$\overline{m}$is the number of edges in $\overline{G}$.

Proof. It is easily seen that

$$\overline{EM_2}(G) = \sum_{uv \notin E(G)} (m+1-(d_G(u)+d_G(v))^2$$

$$= \overline{m}(m+1)^2 + \sum_{uv \notin E(G)} (d_G(u)^2 + d_G(v)^2) - 2(m+1) \sum_{uv \notin E(G)} (d_G(u)+d_G(v))$$

$$= \overline{m}(m+1)^2 + \sum_{uv \notin E(G)} (d_G(u)^2 + d_G(v)^2) + 2\overline{M_2}(G) - 2(m+1)\overline{M_1}(G)$$

as asserted.

Theorem5.*Let G be any nontrivial graph of order n and size m. Then*

$$\overline{EM_2}(G) \leq 2m\Delta'(m+1) - \Delta' M_1(G) - \Delta'\overline{M_2}(G) \quad (8)$$

where Δ' is the maximum degree of an edge.

Proof. Let u and v be any two edges of a graph G. Then $d_{J(G)}(v) = m + 1 - (d_G(u) + d_G(v))$ and let Δ' is the maximum edge degree if a graph G. Then

$$d_G(u)d_G(v) \leq d_G(u)\left(m + 1 - \left(d_G(u) + d_G(v)\right)\right)\Delta'$$

$$\sum_{uv \notin E(G)} (d_G(u)d_G(v)) \leq \sum_{uv \notin E(G)} (d_G(u)\,(m + 1 - (d_G(u) + d_G(v)))\Delta')$$

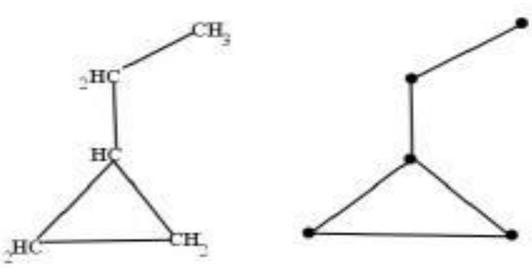
$$\overline{EM_2}(G) \leq \Delta'(m+1)2m - \Delta' M_1(G) - \Delta'\overline{M_2}(G)$$

5. Examples

In this section, we consider some simple molecular graphs and determine their reformulated Zagreb coindices.

Example1.

Consider,ethylcyclopropaneanditscorrespondingmoleculargraphis



ThevaluesofthefirstZagrebindexM_1andthesecondZagrebindexM_2forthegraph representing ethylcyclopropane are $M_1 = 22$and $M_2 = 24$, respectively.The values of thefirstZagrebcoindexandthesecondZagrebcoindexare$\overline{M_1}(G) = 18$ and$\overline{M_2}(G) = 15$ respectively.

Therefore,byProposition1andProposition4,thevaluesofreformulatedfirstand second Zagreb coindex for the molecular graphG representing ethylcyclopropane are

$$\overline{EM_1}(G) = 2\overline{m}(m+1) - 4m(n-1) - 2\,M_1(G)$$

It is easily seen that $m = 5, \overline{m} = 5, n = 5$. Therefore,

$$\overline{EM_1}(G) = 10(5+1) - 20(5-1) - 44 = 24.$$

And

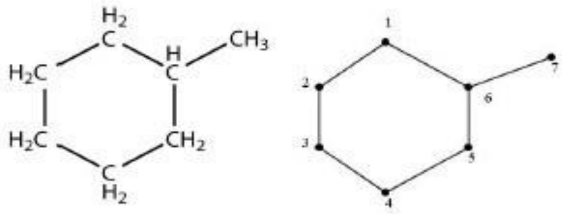
$$\overline{EM_2}(G) = \overline{m}(m+1)^2 + \sum_{uv \notin E(G)} (d_G(u)^2 + d_G(v)^2) + 2\overline{M_2}(G) - 2(m+1)\overline{M_1}(G)$$

$= 5(6)^2 + 36 + 2(6)(18)$

=30.

Example 2.

Consider, methylcyclohexane and its corresponding molecular graph is

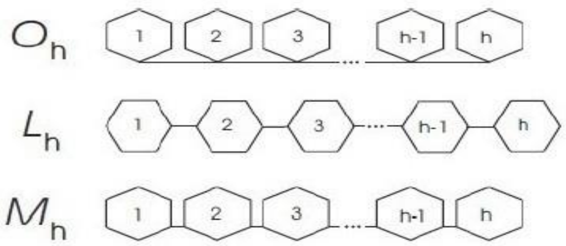


ThevaluesofthefirstZagrebindexM_1andthesecondZagrebindexM_2 forthegraph representing methylcyclohexane are $M_1 = 30$and $M_2 = 31$, respectively.The values of thefirstZagrebcoindexandthesecondZagrebcoindexare$\overline{M_1}(G) = 54$ and$\overline{M_2}(G) = 52$respectively.

Therefore,byProposition1andProposition4,thevaluesofreformulatedfirstand secondZagrebcoindexforthemoleculargraph$G$representingmethylcyclohexaneare $\overline{EM_1}(G) = 98$ and$\overline{EM_2}(G) = 96$.

Example 3.

Two vertices $v$and $w$of a hexagon $H$are said to be in ortho-position if there are adjacent in H.If two vertices $v$and $w$are at distance two then they are said to be in meta-position, and if two vertices $v$and $w$are at distance three then they are said to beinpara-position. Apolyphenylchainof $h$hexagonsisortho-PPC_handisdenotedby O_h,ifallitsinternalhexagonsareotho-hexagons.Infullyanalogusmannaerwedefine meta-$PPC_h$and is denoted by $M_h$and para-$PPC_h$and is denoted by L_h.



The value of first Zagreb index $M_1$is given by $M_1(O_h) = M_1(M_h) = M_1(L_h) = 34h - 10$ see [3].

ThereforebyProposition1,thevalueofreformulatedfirst Zagreb coindex$\overline{EM_1}(G)$is:

$$\overline{EM_1}(G) = 2\overline{m}(m+1) - 4m(n-1) - 2\,M_1(G)$$

$$= 2\overline{m}(m+1) - 4m(n-1) - 68h - 20$$

Refrences

[1] A. R. Ashrafi, T. Došlić, A. Hamzeh, The Zagreb coindices of graph operations, Discrete Appl. Math. 158 (2010) 1571–1578.

[2] A. R. Ashrafi, T. Došlić, A. Hamzeh, Extremalgraphs with respect to the Zagreb coindices, MATCH Commun. Math. Comput.Chem. 65 (2011) 85–92.

[3] M. Azari, Ali Iranmanesh, I. Gutman, Zagreb indices of bridge and chain graphs, MATCH Commun. Math. Comput. Chem. 70 (2013) 921–938.

[4] G. Caporossi, P. Hansen, D. Vukičević, Comparing Zagrebindices of cyclic graphs, MATCH Commun. Math. Comput. Chem. 63 (2010), 441–451.

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

[6] K. C. Das, I. Gutman, B. Zhou, New upper bounds on Zagreb indices, J. Math. Chem. 46 (2009), 514–521.

[7] K.C. Das, I. Gutman, Some properties of the second Zagreb index, MATCH Com- mun. Math. Comput. Chem 52 (2004) 103–112.

[8] T. Došlić, Vertex-weighted Wiener polynomials for composite graphs, ArsMathe-maticaContempooranea 1 (2008) 66–80.

[9] J. B. Diaz, F. T. Metcalf, Stronger forms of a class of inequalities of G. Pólya, G. Szegö and L. V. Kantorovich, Bull. Amer. Math. Soc. 69 (1963) 415-418.

[10] L. Feng, A. Ilić, Zagreb, Harary and hyper-Wiener indices of graphs with a given matching number, Appl. Math. Lett. 23 (2010), 943–948.

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

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

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

[14] F. Harary, Graph Theory, Addison–Wesely, Reading, 1969.

[15] H. Hevia, D. W. VanderJagt, P. Zhang, On the planarity of jump graphs, Discrete Math. 220 (2000) 119-129.

[16] Y. Huang. B. Liu, M. Zhang, On Comparing the variable Zagreb indices, MATCH Commun. Math. Comput. Chem. 63 (2010), 453–460.

[17] A. Ilić, D. Stevanović, On comparing Zagreb indices, MATCH Commun. Math. Comput. Chem. 62 (2009), 681–687.

[18] A. Ilić, B. Zhou, On reformulated Zagreb indices, Discrete Appl. Math. 160 (2012) 204–209.

[19] D. Janežić, A. Miličević, S. Nikolić, N. Trinajstić, Graph-Theoretical Matrices in Chemistry, Mathematical Chemistry Monograph No. 3, edited by I. Gutman, Uni- versty of Kragujevac, Kragujevac, 2007.

[20] M. Liu, B. Liu, New sharp upper bounds for the first Zagreb index, MATCH Com- mun. Math. Comput. Chem. 62 (2009), 689–698.

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

[22] B. Liu, Z. You, A Survey on comparing Zagreb indices, MATCH Commun. Math. Comput. Chem. 65 (2011), 581–593.

[23] M. Liu, A simple approach to order the first Zagreb indices of connected graphs, MATCH Commun. Math. Comput. Chem. 63 (2010), 425–432.

[24] B. Lučić, S. Nokolić, N. Trinajstić, Zagreb indices, In: Chemical Information and Computer Challenges in the 21st Century, edited by M.V. Putz, Nova Sci. Publ., New York, (2012) 261–275.

[25] A. Miličević, S. Nikolić, N. Trinajstić, On reformulated Zagreb indices, Molecular Diversity, 8 (2004) 393–399.

[26] D. S. Mitrinović, P. M. Vasić, Analytic inequalities, Springer-Verlag, Berlin (1970).
[27] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Wiley-VCH, Wein- heim, 2000.
[28] R. Todeschini, V. Consonni, Molecular Descriptors ForChemoinformatics, Wiley- VCH, Weinheim, 2009, Vol. I, Vol. II.
[29] Z. Yan, H. Liu, H. Liu, Sharp bounds for the second Zagreb index of unicyclic graphs, J. Math. Chem. 42 (2007), 565–574.
[30] B. Zhou, I. Gutman, Relations between Wiener, hyper-Wiener and Zagreb indices, Chem. Phys. Lett. 394 (2004), 93–95.
[31] B. Zhou, Upper bounds for the Zagreb indices and the spectral radius of series- parallel graphs, Int. J. Quantum Chem. 107 (2007), 875–878.
[32] B. Zhou, Remarks on Zagreb indices, MATCH Commun. Math. Comput. Chem. 57 (2007), 597–616.
[33] B. Zhou, N. Trinajstić, Some properties of the reformulated Zagreb indices, J. Math Chem 48 (2010) 714–719.