MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **74** (2015) 5-16

ISSN 0340 - 6253

On Zagreb Indices and Coindices

Ivan Gutman[1,2], **Boris Furtula**[1],
Žana Kovijanić Vukićević,[3] **Goran Popivoda**[3]

[1]*Faculty of Science, University of Kragujevac,*
P. O. Box 60, 34000 Kragujevac, Serbia
gutman@kg.ac.rs , furtula@kg.ac.rs

[2]*State University of Novi Pazar, Novi Pazar, Serbia*

[3]*Department of Mathematics, University of Montenegro, P. O. Box 211, 81000 Podgorica, Montenegro*
zanak@t-com.me , goc@t-com.me

(Received January 11, 2015)

Abstract

A complete set of relations is established between the first and second Zagreb index and coindex of a graph and of its complements. Formulas for the first Zagreb index of several derived graphs are also obtained. A remarkable result is that the first Zagreb coindices of a graph and of its complement are always equal.

1 Introduction

The two Zagreb indices belong among the oldest molecular structure descriptors, and their properties have been extensively investigated. Recently, the concept of Zagreb coindices was put forward, attracting much attention of researchers in mathematical chemistry. The aim of the present work is to establish a complete set of relations between Zagreb indices and coindices of graphs and their complements.

In this paper we are concerned with simple graphs, having no directed or weighted edges, and no self loops. Let G be such a graph and let $V(G)$ and $E(G)$ be its vertex and edge sets, respectively. The number of vertices and edges of G will be denoted by

$n = n(G)$ and $m = m(G)$, respectively. In addition, the edge connecting the vertices u and v will be denoted by uv.

The complement $\overline{G}$ of the graph G is the graph with vertex set $V(G)$, in which two vertices are adjacent if and only if they are not adjacent in G.

The degree of the vertex v, denoted by $d_G(v)$, is the number of first neighbors of v in the underlying graph G. Then the first and second Zagreb index are defined as

$$M_1 = M_1(G) = \sum_{v \in V(G)} d_G(v)^2 \tag{1}$$

$$M_2 = M_2(G) = \sum_{uv \in E(G)} d_G(u)\, d_G(v)\,. \tag{2}$$

These topological indices were conceived in the 1970s [13, 15]; for details on their properties and additional references see [4, 9, 10, 12, 14, 21]; for historical details see [11]. In what follows, we need another expression for the first Zagreb index, namely

$$M_1(G) = \sum_{uv \in E(G)} \left[d_G(u) + d_G(v) \right]. \tag{3}$$

The proof of the identity (3) is quite simple. Nevertheless, it seems to be first time mentioned only a few years ago [6].

In 2008, bearing in mind Eq. (3), Došlić put forward the first Zagreb coindex, defined as [6]

$$\overline{M}_1 = \overline{M}_1(G) = \sum_{uv \notin E(G)} \left[d_G(u) + d_G(v) \right]. \tag{4}$$

In view of Eq. (2), the second Zagreb coindex is defined analogously as [6]

$$\overline{M}_2 = \overline{M}_2(G) = \sum_{uv \notin E(G)} d_G(u)\, d_G(v)\,. \tag{5}$$

In Eqs. (4) and (5) is it assumed that $u \neq v$.

The Zagreb coindices were recently studied in some detail [1, 2, 17–19, 22], and the relations between Zagreb indices and coindices were also examined [3, 5, 7, 16, 20].

In this paper, we determine all relations between the Zagreb indices and coindices of a graph G and of its complement $\overline{G}$. In Section 2 we focus our attention to the first Zagreb index, in Section 3 to the second Zagreb index, whereas in Section 4 we obtain relations for the Zagreb indices of certain derived graphs. Not all results outlined in this paper are new, but we state them all for the sake of completeness.

2 Relations for first Zagreb indices and coindices

Theorem 1. *Let G be a graph with n vertices and m edges. Then*

$$M_1(\overline{G}) = M_1(G) + n(n-1)^2 - 4m(n-1) \tag{6}$$

$$\overline{M}_1(G) = 2m(n-1) - M_1(G) \tag{7}$$

$$\overline{M}_1(\overline{G}) = 2m(n-1) - M_1(G)\,. \tag{8}$$

Proof.

Proof of Eq. (7):

We start with the identity

$$\sum_{u\in V(G)} \sum_{v\in V(G)} \big[d_G(u) + d_G(v)\big] = 4mn$$

which is a direct consequence of the fact that the sum of degrees of all vertices is equal to $2m$. The left–hand side summation in the above relation can be partitioned as follows:

$$\sum_{u\in V(G)} \sum_{v\in V(G)} = 2 \sum_{uv\in E(G)} + 2 \sum_{uv\notin E(G)} + 2 \sum_{u=v\in V(G)}$$

which in view of Eqs. (3) and (4) yields

$$\begin{aligned}\sum_{u\in V(G)} \sum_{v\in V(G)} \big[d_G(u) + d_G(v)\big] &= 2\,M_1(G) + 2\,\overline{M}_1(G) + 2 \sum_{v\in V(G)} d_G(v) \\ &= 2\,M_1(G) + 2\,\overline{M}_1(G) + 4m\,.\end{aligned}$$

From

$$2\,M_1(G) + 2\,\overline{M}_1(G) + 4m = 4mn$$

we straightforwardly arrive at Eq. (7).

Proof of Eq. (6):

For any vertex u of the complement $\overline{G}$,

$$d_{\overline{G}}(u) = n - 1 - d_G(u)\,. \tag{9}$$

Bearing in mind Eqs. (3) and (9), we have

$$M_1(\overline{G}) = \sum_{uv\in E(\overline{G})} \big[d_{\overline{G}}(u) + d_{\overline{G}}(v)\big]$$

$$= \sum_{uv\in E(\overline{G})} \big[n-1-d_G(u)+n-1-d_G(v)\big]$$

$$= 2(n-1)\left[\binom{n}{2}-m\right] - \sum_{uv\in E(\overline{G})} \big[d_G(u)+d_G(v)\big]$$

because $\overline{G}$ has $\binom{n}{2}-m$ edges. Now,

$$\sum_{uv\in E(\overline{G})} \big[d_G(u)+d_G(v)\big] = \sum_{uv\notin E(G)} \big[d_G(u)+d_G(v)\big] = \overline{M}_1(G)\,.$$

This yields

$$M_1(\overline{G}) = 2(n-1)\left[\binom{n}{2}-m\right] - \overline{M}_1(G)\,. \tag{10}$$

Substituting Eq. (7) back into (10) yields Eq. (6).

<u>Proof of Eq. (8)</u>:

Using Eqs. (4) and (9), we have

$$\overline{M}_1(\overline{G}) = \sum_{uv\notin E(\overline{G})} \big[d_{\overline{G}}(u)+d_{\overline{G}}(v)\big]$$

$$= \sum_{uv\in E(G)} \big[n-1-d_G(u)+n-1-d_G(v)\big]$$

$$= 2(n-1)m - \sum_{uv\in E(G)} \big[d_G(u)+d_G(v)\big]$$

which in view of Eq. (3) directly leads to Eq. (8). ■

Comparing Eqs. (7) and (8) we arrive at the following surprising conclusion:

Corollary 2. *For any simple graph G,*

$$\overline{M}_1(G) = \overline{M}_1(\overline{G})\,.$$

The Zagreb–index counterpart of Corollary 2 is:

Corollary 3. *Let G be a simple graph with n vertices and m edges. Then*

$$M_1(G) = M_1(\overline{G}) \tag{11}$$

holds if and only if $m = \frac{1}{2}\binom{n}{2}$.

From Corollary 3 it also follows:

Corollary 4. *If Eq. (11) holds, then the number n of vertices satisfies either $n \equiv 0\,(mod\ 4)$ or $n \equiv 1\,(mod\ 4)$.*

Remark 1. *If a graph G is self-complementary (i.e., if $G \cong \overline{G}$), then $m = \frac{1}{2}\binom{n}{2}$ must hold and Eq. (11) is obeyed in a trivial manner. However, there are graphs which are not self-complementary, but for which Eq. (11) holds. The smallest such graphs (with 4 and 5 vertices) are depicted in Fig. 1.*

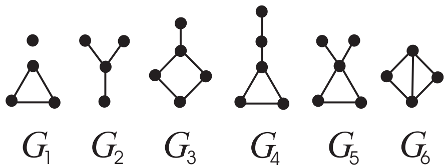

Fig. 1. The smallest non-self-complementary graphs for which Eq. (11) holds. Note that G_2 is the complement of G_1, G_4 is the complement of G_3, and G_6 is the complement of G_5.

3 Relations for second Zagreb indices and coindices

Theorem 5. *Let G be a graph with n vertices and m edges. Then*

$$M_2(\overline{G}) = \frac{1}{2}\,n(n-1)^3 - 3m(n-1)^2 + 2m^2 + \frac{2n-3}{2}\,M_1(G) - M_2(G) \tag{12}$$

$$\overline{M}_2(G) = 2m^2 - \frac{1}{2}\,M_1(G) - M_2(G) \tag{13}$$

$$\overline{M}_2(\overline{G}) = m(n-1)^2 - (n-1)M_1(G) + M_2(G)\,. \tag{14}$$

Proof.

Proof of Eq. (13):

We first note that

$$\sum_{u\in V(G)}\sum_{v\in V(G)} d_G(u)\,d_G(v) = 4m^2\,.$$

The left–hand side summation in the above relation can be partitioned as:

$$\sum_{u\in V(G)}\sum_{v\in V(G)} d_G(u)\,d_G(v) = 2\sum_{uv\in E(G)} d_G(u)\,d_G(v) + 2\sum_{uv\notin E(G)} d_G(u)\,d_G(v) + \sum_{u\in V(G)} d_G(u)^2 = 2\,M_2(G) + 2\,\overline{M}_2(G) + M_1(G)$$

where Eqs. (1), (2), and (5) have been employed. From

$$2\,M_2(G) + 2\,\overline{M}_2(G) + M_1(G) = 4m^2$$

we straightforwardly obtain Eq. (13).

Proof of Eq. (12):

Taking into account relation (9) and the fact that $\overline{G}$ has $\binom{n}{2} - m$ edges, start with Eq. (2) as

$$\begin{aligned}
M_2(\overline{G}) &= \sum_{uv \in E(\overline{G})} d_{\overline{G}}(u)\, d_{\overline{G}}(v) = \sum_{uv \in E(\overline{G})} \big[n-1-d_G(u)\big]\big[n-1-d_G(v)\big] \\
&= (n-1)^2 \sum_{uv \in E(\overline{G})} 1 - (n-1) \sum_{uv \in E(\overline{G})} \big[d_G(u)+d_G(v)\big] + \sum_{uv \in E(\overline{G})} d_G(u)\, d_G(v) \\
&= (n-1)^2 \left[\binom{n}{2} - m\right] - (n-1) \sum_{uv \notin E(G)} \big[d_G(u)+d_G(v)\big] + \sum_{uv \notin E(G)} d_G(u)\, d_G(v) \\
&= (n-1)^2 \left[\binom{n}{2} - m\right] - (n-1)\overline{M}_1(G) + \overline{M}_2(G)\,. \qquad (15)
\end{aligned}$$

Substituting Eqs. (7) and (13) into (15), by a lengthy calculation we obtain Eq. (12).

Proof of Eq. (14):

Using an analogous reasoning, we have

$$\begin{aligned}
\overline{M}_2(\overline{G}) &= \sum_{uv \notin E(\overline{G})} d_{\overline{G}}(u)\, d_{\overline{G}}(v) = \sum_{uv \in E(G)} \big[n-1-d_G(u)\big]\big[n-1-d_G(v)\big] \\
&= (n-1)^2\, m - (n-1) \sum_{uv \in E(G)} \big[d_G(u) + d_G(v)\big] + \sum_{uv \in E(G)} d_G(u)\, d_G(v)
\end{aligned}$$

and Eq. (14) immediately follows. ■

4 Zagreb indices of some derived graphs

In the previous two sections we have shown that if $M_i(G)$, $i = 1, 2$, is known, then also $M_i(\overline{G})$, $\overline{M}_i(G)$, and $\overline{M}_i(\overline{G})$ are known. Therefore, what really needs to be calculated are expressions for $M_1(G)$ and $M_2(G)$. In this section we calculate such expressions for M_1 for a number of familiar derived graphs.

Let, as before, G be a simple graph with n vertices and m edges, with vertex set $V(G)$ and edge set $E(G)$. We are concerned with the following graphs derived from G:

- *Line graph* $L = L(G)$; $V(L) = E(G)$ and two vertices of L are adjacent if the corresponding edges of G are incident.
- *Subdivision graph* $S = S(G)$. $V(S) = V(G) \cup E(G)$ and the vertex of S corresponding to the edge uv of G is inserted in the edge uv of G.
- *Vertex-semitotal graph* $T_1 = T_1(G)$; $V(T_1) = V(G) \cup E(G)$ and $E(T_1) = E(S) \cup E(G)$.
- *Edge-semitotal graph* $T_2 = T_2(G)$; $V(T_2) = V(G) \cup E(G)$ and $E(T_2) = E(S) \cup E(L)$.
- *Total graph* $T = T(G)$; $V(T) = V(G) \cup E(G)$ and $E(T) = E(S) \cup E(G) \cup E(L)$.
- *Paraline graph* $PL = PL(G)$ is the line graph of the subdivision graph.

In Fig. 2 self-explanatory examples of these derived graphs are depicted.

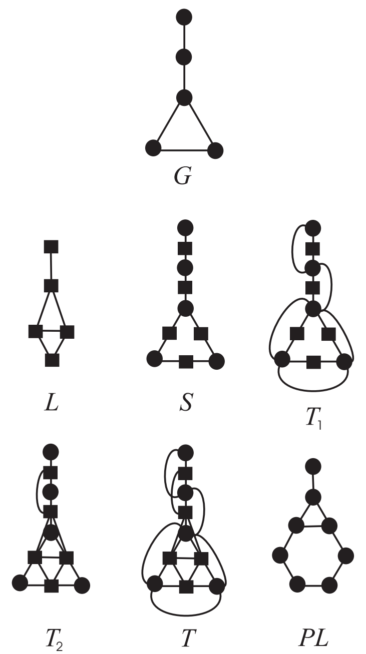

Fig. 2. Various graphs derived from the graph G. The vertices of these derived graphs (except the paraline graph PL), corresponding to the vertices of the parent graph G, are indicated by circles. The vertices of these graphs, corresponding to the edges of the parent graph G are indicated by squares. For details see text.

In order to calculate the first Zagreb index of the above specified derived graphs, we need an auxiliary quantity

$$F = F(G) = \sum_{v \in V(G)} d_G(v)^3 = \sum_{uv \in E(G)} \left[d_G(u)^2 + d_G(v)^2 \right] \tag{16}$$

This vertex–degree–based graph invariant was encountered already in the earliest work on Zagreb indices [15], but was later totally ignored. Only quite recently there has been some interest to it [8]. We prefer to call F the "forgotten topological index".

In what follows, M_1, M_2, and F always refer to the fist Zagreb index, second Zagreb index, and forgotten topological index of the parent graph G.

Proposition 6. *Let L be the line graph of the graph G. Then*

$$M_1(L) = F - 4\,M_1 + 2\,M_2 + 4m\,. \tag{17}$$

Proposition 7. *Let S be the subdivision graph of the graph G. Then*

$$M_1(S) = M_1 + 4m\,. \tag{18}$$

Proposition 8. *Let T_1 be the vertex-semitotal graph of the graph G. Then*

$$M_1(T_1) = 4\,M_1 + 4m\,. \tag{19}$$

Proposition 9. *Let T_2 be the edge-semitotal graph of the graph G. Then*

$$M_1(T_2) = F + M_1 + 2\,M_2\,. \tag{20}$$

Proposition 10. *Let T be the total graph of the graph G. Then*

$$M_1(T) = F + 4\,M_1 + 2\,M_2\,. \tag{21}$$

Proposition 11. *Let PL be the paraline graph of the graph G. Then*

$$M_1(PL) = F\,. \tag{22}$$

Proof. The above defined derived graphs possess vertices corresponding to the vertices of the parent graph G, and vertices corresponding to the edges of the parent graph. The former will be referred to as γ-vertices (in Fig. 2 indicated by circles), whereas the latter as λ-vertices (in Fig. 2 indicated by squares).

Proof of Proposition 6:

The edge uv of the graph G is incident to $d_G(u)+d_G(v)-2$ other edges of G. Therefore,

$$\begin{aligned} M_1(L) &= \sum_{uv\in E(G)} \big[d_G(u)+d_G(v)-2\big]^2 \\ &= \sum_{uv\in E(G)} \big[d_G(u)^2+d_G(v)^2\big] + 2\sum_{uv\in E(G)} d_G(u)\,d_G(v) \\ &- 4\sum_{uv\in E(G)} \big[d_G(u)+d_G(v)\big] + \sum_{uv\in E(G)} 2^2 \end{aligned}$$

which bearing in mind Eqs. (16), (2), and (3), gives Eq. (17).

Proof of Proposition 7:

In the subdivision graph $S(G)$, all γ-vertices have same degree as the corresponding vertices of the parent graph G. All λ-vertices of $S(G)$ are od degree 2. Therefore,

$$M_1(S) = \sum_{v\in V(G)} d_G(v)^2 + \sum_{uv\in E(G)} 2^2$$

which yields Eq. (18).

Proof of Proposition 8:

Observe that in vertex-semitotal graph $T_1(G)$, the degrees of the γ-vertices are equal to twice the degrees of the corresponding vertices of the parent graph G, whereas all λ-vertices are of degree 2. Therefore

$$M_1(T_1) = \sum_{v\in V(G)} \big[2\,d_G(v)\big]^2 + \sum_{uv\in E(G)} 2^2$$

and Eq. (19) follows.

Proof of Proposition 9:

Observe that in the edge-semitotal graph $T_2(G)$, all γ-vertices have same degree as the corresponding vertices of the parent graph G. The degrees of the λ-vertices are by two greater than the degrees of the corresponding vertices in the line graph of G. Bearing this in mind, we have

$$\begin{aligned} M_1(T_2) &= \sum_{v\in V(G)} d_G(v)^2 + \sum_{uv\in E(G)} \big[d(u)+d(v)-2+2\big]^2 \\ &= M_1(G) + \sum_{uv\in E(G)} \big[d(u)^2+d(v)^2\big] + 2\sum_{uv\in E(G)} d(u)\,d(v) \end{aligned}$$

which in view of Eqs. (16) and (2) results in Eq. (20).

Proof of Proposition 10:

In the total graph $T(G)$, the degrees of the γ-vertices are equal to twice the degrees of the corresponding vertices of the parent graph G. The degrees of the λ-vertices are by two greater than the degrees of the corresponding vertices in the line graph of G. Therefore,

$$\begin{aligned} M_1(T) &= \sum_{v\in V(G)} \left[2\,d_G(v)\right]^2 + \sum_{uv\in E(G)} \left[d(u)+d(v)-2+2\right]^2 \\ &= 4\,M_1(G) + \sum_{uv\in E(G)} \left[d(u)^2+d(v)^2\right] + 2\sum_{uv\in E(G)} d(u)\,d(v) \end{aligned}$$

and Eq. (21) follows.

Proof of Proposition 11:

The paraline graph $PL(G)$ of the graph G has $2\,m(G)$ vertices, and the interesting property that $d_G(u)$ of its vertices have the same degree as the vertex u of the parent graph G. Bearing this in mind, we have

$$M_1(PL) = \sum_{x\in V(PL)} d_{PL}(x)^2 = \sum_{u\in V(G)} d_G(u)\left[d_G(u)\right]^2 = \sum_{u\in V(G)} d_G(u)^3 = F(G)$$

which had to be demonstrated. ■

It remains a task for the future to find expressions for the second Zagreb index of the derived graphs considered above.

Remark 2. *A formula equivalent to Eq. (17) was established in [23], pertaining to the "reformulated first Zagreb index". Formula (19) was obtained in [16], where also an incorrect formula (20) was reported.*

Acknowledgement. B. F. thanks the Ministry of Science and Education of Serbia for financial support through the project No. 174033.

References

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

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

[3] J. Baskar Babujee, S. Ramakrishnan, Zagreb indices and coindices for compound graphs, in: R. Nadarajan, R. S. Lekshmi, G. Sai Sundara Krishnan (Eds.), *Computational and Mathematical Modeling*, Narosa, New Delhi, 2012, pp. 357–362.

[4] K. C. Das, I. Gutman, Some properties of the second Zagreb index, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 103–112.

[5] K. C. Das I. Gutman, B. Horoldagva, Comparing Zagreb indices and coindices of trees, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 189–198.

[6] T. Došlić, Vertex–weighted Wiener polynomials for composite graphs, *Ars Math. Contemp.* **1** (2008) 66–80.

[7] T. Došlić, B. Furtula, A. Graovac, I. Gutman, S. Moradi, Z. Yarahmadi, On vertex–degree–based molecular structure descriptors, *MATCH Commun. Math. Comput Chem.* **66** (2011) 613–626.

[8] B. Furtula, I. Gutman, A forgotten topological index, *J. Math. Chem.* **53** (2015) 1184–1190.

[9] B. Furtula, I. Gutman, M. Dehmer, On structure–sensitivity of degree–based topological indices, *Appl. Math. Comput.* **219** (2013) 8973–8978.

[10] I. Gutman, Degree–based topological indices, *Croat. Chem. Acta* **86** (2013) 351–361.

[11] I. Gutman, On the origin of two degree–based topological indices, *Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Natur.)* **146** (2014) 39–52.

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

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

[14] I. Gutman, J. Tošović, Testing the quality of molecular structure descriptors. Vertex–degree–based topological indices, *J. Serb. Chem. Soc.* **78** (2013) 805–810.

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

[16] S. M. Hosamani, I. Gutman, Zagreb indices of transformation graphs and total transformation graphs, *Appl. Math. Comput.* **247** (2014) 1156–1160.

[17] S. Hossein–Zadeh, A. Hamzeh, A. R. Ashrafi, Extermal properties of Zagreb coindices and degree distance of graphs, *Miskolc Math. Notes* **11** (2010) 129–138.

[18] H. Hua, A. Ashrafi, L. Zhang, More on Zagreb coindices of graphs, *Filomat* **26** (2012) 1210–1220.

[19] H. Hua, S. Zhang, Relations between Zagreb coindices and some distance–based topological indices, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 199–208.

[20] Ž. Kovijanić Vukićević, G. Popivoda, Chemical trees with extreme values of Zagreb indices and coindices, *Iran. J. Math. Chem.* **5**(1) (2014) 19–29.

[21] S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, The Zagreb indices 30 years after, *Croat. Chem. Acta* **76** (2003) 113–124.

[22] M. Wang, H. Hua, More on Zagreb coindices of composite graphs, *Int. Math. Forum* **7** (2012) 669–673.

[23] B. Zhou, N. Trinajstić, Some properties of the reformulated Zagreb index, *J. Math. Chem.* **48** (2010) 714–719.