The Zagreb coindices of graph operations

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ARTICLE INFO

Article history:
Received 2 September 2009
Received in revised form 12 May 2010
Accepted 19 May 2010
Available online 29 June 2010

Keywords:
Zagreb coindex
Zagreb index
Product graph

ABSTRACT

Recently introduced Zagreb coindices are a generalization of classical Zagreb indices of chemical graph theory. We explore here their basic mathematical properties and present explicit formulae for these new graph invariants under several graph operations.

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1. Introduction

Chemical graph theory is a branch of mathematical chemistry concerned with the study of chemical graphs. Chemical graphs are models of molecules in which atoms are represented by vertices and chemical bonds by edges of a graph. The basic idea of chemical graph theory is that physico-chemical properties of molecules can be studied by using the information encoded in their corresponding chemical graphs. This information is contained in the adjacency pattern, which is, in turn, dependent on the valences of individual atoms; hence it is inherently local. There are many factors that can contribute to the mechanisms by which the local elements of structure determine various physico-chemical properties of a molecule. Instead of trying to unravel the exact mechanisms, chemical graph theory aims for a less ambitious but a more feasible goal. This is achieved by considering various graph-theoretical invariants of molecular graphs (also known as topological indices or molecular descriptors), and studying how strongly are they correlated with various properties of the corresponding molecules. In this way, chemical graph theory plays an indispensable role in mathematical foundations of the vast area of QSAR (quantitative structure–activity relationship) and QSPR (quantitative structure–property relationship) research.

A graph invariant is any function on a graph that does not depend on a labeling of its vertices. Hundreds of different invariants have been employed to date (with various degrees of success) in QSAR/QSPR studies. We refer the reader to the monograph [21] for a review. Among the more useful invariants there are two that are relevant for the present paper. The pair have been known under various names, but most often as the Zagreb indices. They are defined as sums of contributions dependent on the degrees of adjacent vertices over all edges of a graph. We introduce here a new pair of invariants, the Zagreb coindices, by considering analogous contributions from the pairs of non-adjacent vertices, capturing, thus, and quantifying a possible influence of remote pairs of vertices to the molecule’s properties. The formal definitions of Zagreb coindices and their basic mathematical properties are given in Sections 2 and 3, respectively.

It is well known that many graphs of general, and in particular of chemical, interest arise from simpler graphs via various graph operations. It is, hence, important to understand how certain invariants of such composite graphs are related to the corresponding invariants of their components. Graovac and Pisanski [6] were the first to consider the problem of
computing topological indices of product graphs. In their paper, they computed an exact formula for the Wiener index of the Cartesian product of graphs. The results were generalized by a series of authors who computed unweighted and vertex-weighted Wiener (or Hosoya) polynomials for various classes of composite graphs \cite{19,20,4}, including the Cartesian product, composition, sum, disjunction and symmetric difference of two graphs. Then, Klavžar et al. \cite{15,16} computed the Szeged index of Cartesian product graphs and presented some partial works on other graph operations. In a series of recent papers \cite{9–14,24}, one of the present authors (ARA) and his coworkers extended this program to other topological indices, such as the vertex and edge PI index, the vertex and edge versions of Szeged index, the first and second Zagreb index, and the hyper-Wiener and the edge-Wiener indices of several operations. Here we continue this line of research by exploring the behavior of Zagreb coindices under several important binary operations. The operations are reviewed in Section 4, and for all of them the explicit formulae for Zagreb coindices of composite graphs are given. The results are applied to several classes of chemically interesting graphs, such as nanotubes, nanotori, and various linear polymers.

2. Zagreb indices and Zagreb coindices

All graphs in this paper are finite and simple. For terms and concepts not defined here we refer the reader to any of several standard monographs such as, e.g., \cite{3,7,22} or \cite{23}.

Let $G$ be a finite simple graph on $n$ vertices and $m$ edges. We denote the vertex and the edge set of $G$ by $V(G)$ and $E(G)$, respectively. The \textbf{complement} of $G$, denoted by $\overline{G}$, is a simple graph on the same set of vertices $V(G)$ in which two vertices $u$ and $v$ are adjacent, i.e., connected by an edge $uv$, if and only if they are not adjacent in $G$. Hence, $uv \in E(\overline{G}) \iff uv \notin E(G)$. (Notice that this definition excludes loops in $G$.) Obviously, $E(G) \cup E(\overline{G}) = E(K_n)$, and $\overline{m} = |E(\overline{G})| = \binom{n}{2} - m$. The degree of a vertex $u$ in $G$ is denoted by $d(u)$; the degree of the same vertex in $\overline{G}$ is then given by $\overline{d}(u) = n - 1 - d(u)$. We will omit the subscript $G$ when the graph is clear from the context.

The \textbf{Zagreb indices} were originally defined as follows.

$$M_1(G) = \sum_{u \in V(G)} d(u)^2; \quad M_2(G) = \sum_{u \in V(G)} d(u)d(v).$$

Here $M_1(G)$ and $M_2(G)$ denote the first and the second Zagreb index, respectively. The first Zagreb index can also be expressed as a sum over edges of $G$,

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

We refer the reader to \cite{18} for the proof of this fact and for more information on Zagreb indices.

The Zagreb indices can be viewed as the contributions of pairs of adjacent vertices to additively and multiplicatively weighted versions of Wiener numbers and polynomials \cite{17}. Curiously enough, it turns out that similar contributions of \textbf{non-adjacent} pairs of vertices must be taken into account when computing the weighted Wiener polynomials of certain composite graphs \cite{4}. As the sums involved run over the edges of the complement of $G$, such quantities were called Zagreb coindices. More formally, the \textbf{first Zagreb coindex} of a graph $G$ is defined as

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

and the \textbf{second Zagreb coindex} of a graph $G$ is given by

$$\overline{M}_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

The pair of new invariants was formally introduced in \cite{4} in the hope that it will improve our ability to quantify the contributions of pairs of non-adjacent vertices to various properties of molecules. As a bonus, the new invariants allowed for more compact expressions for the vertex-weighted Wiener polynomials of the considered composite graphs. For some recent results on the extremal values of Zagreb coindices over several classes of graphs, we refer the reader to \cite{1}.

The reader should note that Zagreb coindices of $G$ are not Zagreb indices of $\overline{G}$; the defining sums run over $E(\overline{G})$, but the degrees are with respect to $G$. However, those quantities are closely related. We explore the case of $\overline{M}_1(G)$ first.

3. Basic properties of Zagreb coindices

\textbf{Proposition 1.} Let $G$ be a simple graph on $n$ vertices and $m$ edges. Then $M_1(\overline{G}) = M_1(G) + 2(n - 1)(\overline{m} - m)$.

\textbf{Proof.}

$$M_1(\overline{G}) = \sum_{u \in V(G)} \overline{d}(u)^2 = \sum_{u \in V(G)} [n - 1 - d_c(u)]^2$$

$$= \sum_{u \in V(G)} (n - 1)^2 - 2(n - 1) \sum_{u \in V(G)} d_c(u) + \sum_{u \in V(G)} d_c(u)^2$$

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

\square
Proposition 2. Let $G$ be a simple graph on $n$ vertices and $m$ edges. Then $\overline{M}_1(G) = 2m(n-1) - M_1(G)$.

Proof.
\[
\overline{M}_1(G) = \sum_{uv \notin E(G)} [d(u) + d(v)]
\]
\[
= \sum_{uv \notin E(G)} [2(n-1) - (d_G(u) + d_G(v))]
\]
\[
= 2(n-1)m - M_1(\overline{G}) = 2m(n-1) - M_1(G). \quad \square
\]

The result of Proposition 2 was also obtained by Das and Gutman in a paper about Zagreb indices [2].

By writing Proposition 1 as $M_1(G) = M_1(\overline{G}) = 2(n-1)(\overline{m} - m)$, one can see that the first Zagreb index of a graph will coincide with the first Zagreb index of its complement if and only if the graph and the complement have the same number of edges. A stronger claim turns out to be true for the first Zagreb coindex.

Proposition 3. Let $G$ be a simple graph. Then $\overline{M}_1(G) = \overline{M}_1(\overline{G})$.

Proof. By applying Proposition 2 to $\overline{G}$, one obtains $\overline{M}_1(\overline{G}) = 2\overline{m}(n-1) - M_1(\overline{G})$. Now, plugging in the expression for $M_1(\overline{G})$ from Proposition 1 yields
\[
\overline{M}_1(\overline{G}) = 2\overline{m}(n-1) - M_1(G) - 2(n-1)(\overline{m} - m),
\]
and this is exactly the expression for $\overline{M}_1(G)$ from Proposition 2. Hence $\overline{M}_1(G) = \overline{M}_1(\overline{G})$ for all simple graphs $G$. \quad \square

The expressions for $\overline{M}_2(G)$ are less elegant than those for $\overline{M}_1(G)$. The following was obtained by Das and Gutman in [2].

Proposition 4. Let $G$ be a simple graph on $n$ vertices and $m$ edges. Then
\[
\overline{M}_2(G) = 2m^2 - M_2(G) - \frac{1}{2}M_1(G). \quad \square
\]

The result follows by squaring both sides of the identity $\sum_{uv \in V(G)} d(u) = 2m$ and then splitting the term $2 \sum d(u)d(v)$ into two sums, one over the edges of $G$, and the other over the edges of $\overline{G}$.

An alternative expression for $\overline{M}_2(G)$ can be obtained by changing the signs of both terms in the product contributed by each of the missing edges.

Proposition 5. Let $G$ be a simple graph on $n$ vertices and $m$ edges. Then
\[
\overline{M}_2(G) = M_2(\overline{G}) - (n-1)M_1(\overline{G}) + \overline{m}(n-1)^2.
\]

Proof.
\[
\overline{M}_2(G) = \sum_{uv \notin E(G)} d(u)d(v)
\]
\[
= \sum_{uv \notin E(G)} [-d(u)][-d(v)]
\]
\[
= \sum_{uv \notin E(G)} [n - d(u) - 1 - (n-1)][n - d(v) - 1 - (n-1)]
\]
\[
= M_2(\overline{G}) - (n-1)M_1(\overline{G}) + \overline{m}(n-1)^2. \quad \square
\]

It follows directly from the definitions that both Zagreb coindices achieve their smallest possible value of zero on complete and on empty graphs. In the case of complete graphs, the sums are taken over the empty set of edges; in the case of empty graphs, all degrees are zero.

Proposition 6.
\[
\overline{M}_1(K_n) = \overline{M}_1(\overline{K}_n) = 0;
\]
\[
\overline{M}_2(K_n) = \overline{M}_2(\overline{K}_n) = 0. \quad \square
\]

The following results for paths and cycles on $n$ vertices follow easily by direct calculations.

Proposition 7.
\[
\overline{M}_1(P_n) = 2(n-2)^2;
\]
\[
\overline{M}_2(P_n) = 2n^2 - 10n + 13;
\]
\[
\overline{M}_1(C_n) = \overline{M}_2(C_n) = 2n(n - 3). \quad \square
\]
4. Main results

In this section, we introduce the graph operations used for producing the composite graphs that are relevant for our purpose and review their basic properties. We consider seven operations. Each of them is treated in a separate subsection. The order of subsections is determined by the increasing complexity of presented results. We refer the reader to monograph [8] for more information on composite graphs.

All considered operations are binary. Hence, we will usually deal with two finite and simple graphs, $G_1$ and $G_2$. For a given graph $G_i$, its vertex and edge sets will be denoted by $V_i$ and $E_i$, respectively, and their cardinalities by $n_i$ and $m_i$, respectively, where $i = 1, 2$. The number of edges in $G_i$ is denoted by $m_i$. When more than two graphs can be combined using a given operation, the values of subscripts will vary accordingly.

4.1. Union

The simplest operation we consider here is a union of two graphs. A union $G_1 \cup G_2$ of the graphs $G_1$ and $G_2$ is the graph with the vertex set $V_1 \cup V_2$ and the edge set $E_1 \cup E_2$. Here we assume that $V_1$ and $V_2$ are disjoint.

**Proposition 8.** Let $G_1$ and $G_2$ be two simple graphs. Then

(i) $M_1(G_1 \cup G_2) = M_1(G_1) + M_1(G_2) + 2(m_1n_2 + m_2n_1);$

(ii) $M_2(G_1 \cup G_2) = M_2(G_1) + M_2(G_2) + 4m_1m_2.$

**Proof.** The degree $d_{G_1 \cup G_2}(u)$ of a vertex $u$ is equal to the degree of $u$ in the component $G_i$ that contains it. The first Zagreb coindex of $G_1 \cup G_2$ is then equal to the sum of the first Zagreb coindices of the components plus the contributions from the missing edges between the components. But the missing edges make the edge set of $K_{n_1,n_2}$; hence there are $n_1n_2$ of them, and their total contribution is given by

$$\sum_{u \in V(G_1)} \left[ \sum_{v \in V(G_2)} (d(u) + d(v)) \right] = \sum_{u \in V(G_1)} [n_2d(u) + 2m_2] = 2(m_1n_2 + m_2n_1).$$

This gives us the first claim. The second claim follows by the same reasoning, since the contribution of the missing edges between $G_1$ and $G_2$ is given by

$$\sum_{u \in V(G_1)} \left[ \sum_{v \in V(G_2)} d(u)d(v) \right] = \sum_{u \in V(G_1)} d(u) \sum_{v \in V(G_2)} d(v) = 4m_1m_2. \quad \Box$$

The established formulae for the Zagreb coindices of union will be useful when considering more complex operations. They can be generalized to the case of a union of more than two graphs in a straightforward manner, and we leave that to the interested reader.

4.2. Sum (join)

Next in the order of complexity is the operation of sum of two graphs. A sum $G_1 + G_2$ of two graphs $G_1$ and $G_2$ with disjoint vertex sets $V_1$ and $V_2$ is the graph on the vertex set $V_1 \cup V_2$ and the edge set $E_1 \cup E_2 \cup \{u_1u_2; u_1 \in V_1, u_2 \in V_2\}$. Hence, the sum of two graphs is obtained by connecting each vertex of one graph to each vertex of the other graph, while keeping all edges of both graphs. The sum of two graphs is sometimes also called a join, and is denoted by $G_1 \nabla G_2$. We first consider the case where one of the components in a sum is single vertex.

**Proposition 9.** (i) $M_1(G + K_1) = M_1(G) + 2\overline{m};$

(ii) $M_2(G + K_1) = M_2(G) + M_1(G) + \overline{m}.$

**Proof.** The first claim follows from the relation $G + K_1 = \overline{G} \cup K_1$ by using Propositions 3 and 8(i). To prove the second claim, we consider

$$M_2(G + K_1) = \sum_{u_1 \neq u_2 \in V(G)} d(u_1)d(u_2) + \sum_{u \in V(G) \setminus \{V(K_1)\}} d(u) \cdot n.$$

But the second sum on the right-hand side runs over the empty set of edges; hence, it is equal to zero. The degrees in the remaining sum are taken with respect to the whole graph $G + K_1$. Hence, $d(u_i) = d_C(u_i) + 1$ for $i = 1, 2$. Now, we have

$$M_2(G + K_1) = \sum_{u_1 \neq u_2 \in V(G)} [d_C(u_1) + 1][d_C(u_2) + 1]$$

$$= \sum_{u_1 \neq u_2 \in V(G)} d_C(u_1)d_C(u_2) + \sum_{u_1 \neq u_2 \in V(G)} [d_C(u_1) + d_C(u_2)] + \sum_{u_1 \neq u_2 \in V(G)} 1$$

$$= M_2(G) + M_1(G) + \overline{m}. \quad \Box$$
From Proposition 9, we obtain explicit formulae for the Zagreb coinides of the $n$-vertex star $S_n = K_{1,n-1} = \overline{K}_{n-1} + K_1$ for $n \geq 2$.

\[
\begin{align*}
\overline{M}_1(S_n) &= (n-1)(n-2); \\
\overline{M}_2(S_n) &= \left( \frac{n-1}{2} \right).
\end{align*}
\]

Now we tackle the general case.

**Proposition 10.** Let $G_1$ and $G_2$ be two simple graphs. Then

(i) $\overline{M}_1(G_1 + G_2) = \overline{M}_1(G_1) + \overline{M}_1(G_2) + 2(\overline{m}_1n_2 + \overline{m}_2n_1)$;

(ii) $\overline{M}_2(G_1 + G_2) = \overline{M}_2(G_1) + \overline{M}_2(G_2) + n_1\overline{M}_1(G_1) + n_1\overline{M}_1(G_2) + \overline{m}_1n_2^2 + \overline{m}_2n_1^2$.

**Proof.** The first claim again follows from Proposition 9. To prove the second claim, notice that $d_{G_1 + G_2}(u) = d_{G_1}(u) + n_2$, and $d_{G_1 + G_2}(v) = d_{G_2}(v) + n_1$ for $u \in V(G_1)$, $v \in V(G_2)$. Since all possible edges between $G_1$ and $G_2$ are present in $G_1 + G_2$, there are no missing edges, and hence their contribution is zero. The remaining two contributions, one from the edges missing in $G_1$ and the other from the edges missing in $G_2$, are given by

\[
\sum_{e \in \overline{E}(G_1)} [(d_{G_1}(u) + n_2)(d_{G_2}(v) + n_2)] = \overline{M}_2(G_1) + n_2\overline{M}_1(G_1) + n_2^2\overline{m}_1,
\]

and similarly for the sum over the edges missing in $G_2$. Claim (ii) now follows by adding the two contributions. \(\square\)

Now we can give the explicit formulae for $\overline{M}_1(K_{p,q})$ and $\overline{M}_2(K_{p,q})$ for $p, q \geq 2$. They follow from $K_{p,q} = \overline{K}_p + \overline{K}_q$ via Proposition 9.

**Corollary 11.** (i) $\overline{M}_1(K_{p,q}) = pq(p + q - 2)$;

(ii) $\overline{M}_2(K_{p,q}) = \frac{1}{2}pq(2pq - (p + q))$. \(\square\)

The sum operation can be extended inductively to more than two graphs in an obvious way. Let $G_1, \ldots, G_k$ be graphs with vertex sets $V_i$ and edge sets $E_i$ of cardinality $n_i$ and $m_i$, respectively. Their sum is a graph $G_1 + \cdots + G_k$ on the vertex set $V_1 \cup \cdots \cup V_k$ and the edge set $E_1 \cup \cdots \cup E_k \cup \{v_i|v_i \in V_i, v_j \in V_j, i \neq j\}$. Starting from Proposition 10, by inductive reasoning we obtain the following expression for the first Zagreb coindex of a sum of several graphs.

**Corollary 12.**

\[
\overline{M}_1(G_1 + \cdots + G_k) = \sum_{i=1}^k \overline{M}_1(G_i) + 2 \sum_{i=1}^k \left[ n_i \left( \sum_{j=1}^k \overline{m}_j - \overline{m}_i \right) \right]. \quad \square
\]

As an illustration, we consider the case of the complete $k$-partite graph $K_{n_1, \ldots, n_k}$ with classes of partitions of sizes $n_1, \ldots, n_k$. This graph is a sum of $k$ empty graphs $\overline{K}_{n_i}$, and from Corollary 11 we can easily obtain a formula for $\overline{M}_1(K_{n_1, \ldots, n_k})$ by noting that the first sum of the right-hand side is equal to zero. A particularly simple formula is obtained when all classes are of equal size, say $p$. In this case, we have a balanced complete $k$-partite graph on $k \cdot p$ vertices, and its first Zagreb coindex is given by

\[
\overline{M}_1(K_{p,\ldots,p}) = 4p \left( \binom{p}{2} \right)^k \binom{k}{2}.
\]

The above formula can be also verified by direct computation.

### 4.3. Cartesian product

Now we consider a series of four operations – Cartesian product, disjunction, symmetric difference and composition – that result in a graph defined on the Cartesian product of vertex sets of participating graphs. All four are associative, and the composition is the only one that is not commutative. The shared properties make the first three operations suitable for a syoptic treatment. As the Cartesian product is the most important of them, we use it as a representative of the whole group and present the results in more detail.

For given graphs $G_1$ and $G_2$, we define their **Cartesian product** $G_1 \square G_2$ as the graph on the vertex set $V(G_1) \times V(G_2)$ with vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ connected by an edge if and only if $[u_1 = v_1$ and $[u_2, v_2] \in E(G_2)]$ or $[u_2 = v_2$ and $[u_1, v_1] \in E(G_1)]$. Obviously, $|E(G_1 \square G_2)| = n_1m_2 + n_2m_1$, where $n_1$ and $m_1$ denote the number of vertices and edges, respectively, of $G_1$. The degree of a vertex $(u_1, u_2)$ of $G_1 \square G_2$ is obtained by adding the degrees of its projections to the respective components, $d_{G_1 \square G_2}(u_1, u_2) = d_{G_1}(u_1) + d_{G_2}(u_2)$. The Cartesian product of two graphs is connected if and only if both components are connected.
Proposition 13.
\[
\begin{align*}
\overline{M}_1(G_1 \Box G_2) &= 2(n_1m_2 + n_2m_1)(n_1n_2 - 1) - 8m_1m_2 - n_1M_1(G_1) - n_1M_1(G_2) \\
\overline{M}_2(G_1 \Box G_2) &= 2(n_1m_2 + n_2m_1)^2 - 4m_1m_2 - [n_1M_2(G_2) + n_2M_2(G_1)] \\
&\quad - \left[3m_2 + \frac{1}{2}n_2\right] M_1(G_1) + \left[3m_1 + \frac{1}{2}n_1\right] M_1(G_2).
\end{align*}
\]

Proof. The first formula follows from Proposition 2 and the expression \(M_1(G_1 \Box G_2) = n_2M_1(G_1) + n_1M_1(G_2) + 8m_1m_2\) from Theorem 1 of [11]. The second formula follows in the same way by plugging the expression \(M_2(G_1 \Box G_2) = n_1M_2(G_2) + n_2M_2(G_1) + 3m_2M_1(G_1) + 3m_1M_1(G_2)\) from Theorem 4 of [11] into Proposition 4.

As an application of the above result, we list explicit formulae for the first Zagreb coindex of \(P_i \Box P_j, P_i \Box C_q\) and \(C_p \Box C_q\). These graphs are known as the rectangular grid, the \(C_q\) nanotube, and the \(C_p\) nanotorus, respectively. The formulae follow from Proposition 13 by plugging in the expressions \(M_1(P_n) = 4n - 6\) and \(M_1(C_n) = 4n\).

Corollary 14. \(\overline{M}_1(P_i \Box P_j) = 2(2rs - r + s - 10) + 4(2r + s - 1)\); \(\overline{M}_1(P_i \Box C_q) = 2q(2qr^2 - qr - 10r + 8)\); \(\overline{M}_1(C_p \Box C_q) = 4pq(pq - 5)\).

Similar formulae can be obtained for the second Zagreb coindex of the above graphs by taking into account the expressions \(M_2(P_i) = 4(n - 2)\) for \(n \geq 3\), \(M_2(P_2) = 1\), and \(M_2(C_n) = 4n\). Particularly simple is the expression for the nanotorus case, \(\overline{M}_2(C_p \Box C_q) = 8pq(pq - 3)\). Further results can be obtained for ladders and prisms by specializing the value of \(r\) to 2 in the above formulæ, but we leave this to the reader.

The Cartesian product is defined for more than two graphs in an obvious manner. If \(G_1, \ldots, G_k\) are some graphs, the first Zagreb index of their product \(\prod_{i=1}^k G_i\) is given by
\[
\overline{M}_1(\prod_{i=1}^k G_i) = \prod_{i=1}^k \left(\frac{M_1(G_i)}{n_i} + 4 \sum_{i,j=1}^k \frac{m_i m_j}{n_i n_j}\right).
\]
(We refer the reader to [11] for the proof of this result and also for similar but more complicated expression for the \(M_2(\prod_{i=1}^k G_i)\). By plugging this into Proposition 2, one can obtain the expression for \(\overline{M}_1(\prod_{i=1}^k G_i)\) in terms of the first Zagreb index of the factors. In the simplest situation, when all factors are equal, we obtain a formula for the first Zagreb coindex of \(k\)-th Cartesian power of a graph \(G\).

Corollary 15. \(\overline{M}_1(\Box^k k) = kn^{k-2}[2mn(n^k - 1) - nM_1(G) - 4(k - 1)m^2]\).

As an application, we present the formula for \(\overline{M}_1(Q_k)\), where \(Q_k = (K_2)^k\) is the \(k\)-dimensional hypercube.
\[
\overline{M}_1(Q_k) = k2^k(2^k - k - 1).
\]

4.4. Disjunction

The disjunction \(G_1 \lor G_2\) of two graphs \(G_1\) and \(G_2\) is the graph with vertex set \(V(G_1) \times V(G_2)\) in which \((u_1, u_2)\) is adjacent with \((v_1, v_2)\) whenever \(u_1\) is adjacent with \(v_1\) in \(G_1\) or \(u_2\) is adjacent with \(v_2\) in \(G_2\). The degree of a vertex \((u_1, u_2)\) of \(G_1 \lor G_2\) is given by \(d_{G_1 \lor G_2}(u_1, u_2) = n_2d_{G_1}(u_1) + n_1d_{G_2}(u_2) - d_{G_1}(u_1)d_{G_2}(u_2)\), while the number of edges of \(G_1 \lor G_2\) is equal to \(n_1^2m_2 + n_2^2m_1 - 2m_1m_2\).

Proposition 16.
\[
\overline{M}_1(G_1 \lor G_2) = 4m_1m_2(1 - 3n_1n_2) + 2n_1n_2(n_1^2m_2 + n_2^2m_1) - 2(n_1^2m_2 + n_2^2m_1) \\
+ n_2(4m_2 - n_1n_2)M_1(G_1) + n_1(4m_1 - n_1n_2)M_1(G_2) - M_1(G_1)M_1(G_2).
\]

The proof follows by combining Proposition 2 with the relevant results from [11], and we omit it. By the same reasoning, one can obtain a formula for \(\overline{M}_2(G_1 \lor G_2)\), but it is too cumbersome to be of much practical interest and we do not present it here.

4.5. Symmetric difference

The symmetric difference \(G_1 \oplus G_2\) of two graphs \(G_1\) and \(G_2\) is the graph with vertex set \(V(G_1) \times V(G_2)\) in which \((u_1, u_2)\) is adjacent with \((v_1, v_2)\) whenever \(u_1\) is adjacent with \(v_1\) in \(G_1\) or \(u_2\) is adjacent with \(v_2\) in \(G_2\), but not both. The degree of a vertex \((u_1, u_2)\) of \(G_1 \oplus G_2\) is given by \(d_{G_1 \oplus G_2}(u_1, u_2) = n_2d_{G_1}(u_1) + n_1d_{G_2}(u_2) - 2d_{G_1}(u_1)d_{G_2}(u_2)\), while the number of edges in \(G_1 \oplus G_2\) is \(n_1^2m_2 + n_2^2m_1 - 4m_1m_2\).
Much as in the previous case, we present only the formula for the first Zagreb coindex of a symmetric difference of two graphs.

**Proposition 17.**

\[ \overline{M}_1(G_1 \oplus G_2) = 2(n_1n_2 - 1)(n_1^2m_2 + n_2^2m_1) + 8m_1m_2(1 - 2n_1n_2) + n_2(8m_2 - n_1n_2) + n_1(8m_1 - n_1n_2)M_1(G_1) - 4M_1(G_1)M_1(G_2). \]

4.6. Composition

The composition \(G_1[G_2]\) of graphs \(G_1\) and \(G_2\) with disjoint vertex sets and edge sets is again a graph on vertex set \(V(G_1) \times V(G_2)\) in which \(u = (u_1, u_2)\) is adjacent with \(v = (v_1, v_2)\) whenever \([u_1\text{ is adjacent with }v_1]\) or \([u_1 = v_1\text{ and }u_2\text{ is adjacent with }v_2]\). The composition is not commutative. The easiest way to visualize the composition \(G_1[G_2]\) is to expand each vertex of \(G_1\) into a copy of \(G_2\), with each edge of \(G_1\) replaced by the set of all possible edges between the corresponding copies of \(G_2\). Hence the number of edges in \(G_1[G_2]\) is given by \(|E(G_1[G_2])| = n_1m_2 + n_2m_1^2\). The degree of a vertex \((u_1, u_2)\) of \(G_1[G_2]\) is given by \(d_{G_1[G_2]}((u_1, u_2)) = n_2d_{G_1}(u_1) + d_{G_2}(u_2)\).

**Proposition 18.**

\[ \overline{M}_1(G_1[G_2]) = 2n_1n_2(n_1m_2 + n_2m_1) - 2m_1(n_1 + n_2^2) - 8n_2m_1m_2 - n_2^2M_1(G_1) - n_1M_1(G_2); \]
\[ \overline{M}_2(G_1[G_2]) = 2m_2n_2^2 + 2m_2n_1 + 2m_2n_1^2 - 4m_1m_2(n_2 + m_2) - n_2^2\left(3m_2 + n_2^2\right)M_1(G_1) - \left(n_1^2 + 2n_2m_1\right)M_1(G_2) - (n_2^2M_2(G_1) + n_1M_2(G_2)). \]

The proof follows much in the same way as in the previous cases, and we omit it. As an application we present formulae for Zagreb coindices of open and closed fences, \(P_n[K_2]\) and \(C_n[K_2]\).

**Corollary 19.**

\[ \overline{M}_1(P_n[K_2]) = 18(n - 2)^2; \]
\[ \overline{M}_2(P_n[K_2]) = 50n^2 - 230n + 276; \]
\[ \overline{M}_1(C_n[K_2]) = 2n(9n - 29); \]
\[ \overline{M}_2(C_n[K_2]) = 50n(n - 3). \]

4.7. Corona

For given graphs \(G_1\) and \(G_2\), we define their corona product \(G_1 \circ G_2\) as the graph obtained by taking \(|V(G_1)|\) copies of \(G_2\) and joining each vertex of the \(i\)-th copy with vertex \(v_i \in V(G_1)\). Obviously, \(|V(G_1 \circ G_2)| = n_1(1 + n_2)\) and \(|E(G_1 \circ G_2)| = m_1 + n_1(n_2 + m_2)\).

The vertex set of a corona product of two graphs is not the Cartesian product of their vertex sets. However, each vertex \(v\) of a copy of \(G_2\) attached to a vertex \(u\) from \(G_1\) can be uniquely described by the ordered pair \((u, v)\). Hence the vertices in all copies of \(G_2\) can be described as the elements of the Cartesian product \(V(G_1) \times V(G_2)\). This description can be extended to all vertices of \(G_1 \circ G_2\) by introducing a special symbol \(\phi\) so that \(V(G_1 \circ G_2) = V(G_1) \times (V(G_2) \cup \{\phi\})\), where ordered pairs \((u, \phi)\) denote the vertices of \(G_1\). It follows from the definition that by forming a corona product \(G_1 \circ G_2\) each vertex of \(G_1\) gets \(|V(G_2)| = n_2\) new neighbors; hence the degree of a vertex \(u \in V(G_1)\) in \(G_1 \circ G_2\) is given by \(d_{G_1 \circ G_2}(u) = d_{G_1}(u) + n_2\). Similarly, the degree of each vertex in a copy of \(G_2\) will increase by one. Hence,

\[ d_{G_1 \circ G_2}(u, v) = \begin{cases} d_{G_1}(u) + n_2 & \text{if } v = \phi; \\ d_{G_2}(v) + 1 & \text{if } v \in V(G_2). \end{cases} \]

**Proposition 20.**

\[ \overline{M}_1(G_1 \circ G_2) = \overline{M}_1(G_1) + n_1\overline{M}_1(G_2) + 2[n_1(\overline{m}_2 - m_2) + n_2(\overline{m}_1 - m_1)] + 2m_2n_1^2 + n_1n_2[2(m_2 + n_2)(n_1 - 1) + n_1 + 2m_1 - 1]; \]
\[ \overline{M}_2(G_1 \circ G_2) = \overline{M}_2(G_1) + n_1\overline{M}_2(G_2) + n_1[\overline{M}_1(G_2) + \overline{M}_2(G_2)] + n_2^2\overline{m}_1 + n_1\overline{m}_2 + n_1n_2 \left(4n_1m_2 + \frac{3}{2}n_1n_2 - 4m_2 - \frac{3}{2}n_2\right) + (n_1 - 1)(4m_1m_2 + 2n_2m_1 + 2m_2^2n_1). \]

The proof follows by manipulating the defining formulae, and we omit it. As an application of this result, we present the formulae for Zagreb coindices of a thorny cycle \(C_n \circ K_\ell\).
Corollary 21.

\[
\begin{align*}
\overline{M}_1(C_n \circ K_k) &= nk(2nk + 4n - k - 7) + 2n(n - 3); \\
\overline{M}_2(C_n \circ K_k) &= \frac{1}{2} n(k + 1)[4n(k + 1) - 5k - 12].
\end{align*}
\]

\[\Box\]

5. Concluding remarks

Zagreb coindices are a pair of recently introduced graph invariants that generalize much used Zagreb indices. In this paper we have investigated their basic mathematical properties and obtained explicit formulae for their values under several graph operations. However, much work still needs to be done, and here we mention some possible directions for future research.

In order to keep this paper to a reasonable length, it was necessary to leave out some operations, such as splices and links of two or more graphs, for example. Both operations are of considerable chemical interest [5]. By their iteration we arrive at various types of linear polymers. It would be interesting to have explicit or at least recursive formulae for their Zagreb coindices. Another problem worth looking at is to determine extremal values of Zagreb coindices over various classes of graphs. For some initial progress in that direction we refer the reader to [1]. While the extremal values over all trees can be easily derived from the presented results, the problem is unsolved for the class of chemical trees. Finally, one could also look at the behavior of Zagreb coindices under various local operations such as edge deletions, contractions and subdivisions, for example.

Acknowledgements

Partial support of the Ministry of Science, Education and Sport of the Republic of Croatia (Grants No. 037-0000000-2779 and 177-0000000-0884) is gratefully acknowledged. The first author was supported in part by a grant from IPM (No.87200113).

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