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A new version of Zagreb indices

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Abstract

The Zagreb indices have been introduced by Gutman and Trinajstić as $M_1(G) = \sum_{v \in V(G)} (d_G(v))^2$ and $M_2(G) = \sum_{uv \in E(G)} d_G(u)d_G(v)$, where $d_G(u)$ denotes the degree of vertex u. We now define a new version of Zagreb indices as $M_1^*(G) = \sum_{uv \in E(G)} [\varepsilon_G(u) + \varepsilon_G(v)]$ and $M_2^*(G) = \sum_{uv \in E(G)} \varepsilon_G(u)\varepsilon_G(v)$, where $\varepsilon_G(u)$ is the largest distance between u and any other vertex v of G. The goal of this paper is to further the study of these new topological index.

1 Introduction

A *graph* is a collection of points and lines connecting a subset of them. The points and lines of a graph are also called vertices and edges of the graph, respectively. The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. A *molecular graph* is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Note that hydrogen atoms are often omitted. *Chemical graph theory* is a branch of mathematical chemistry which has an important effect on the development of the chemical sciences.

By IUPAC terminology, a *topological index* is a numerical value associated with chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. In an exact phrase, if *Graph* denotes the class of all finite graphs then a topological index is a function *Top* from *Graph* into real numbers with this property that $Top(G) = Top(H)$, if G and H are isomorphic. Obviously, the number of vertices and the number of edges are topological index. The *Wiener* index [13] is the first reported distance based topological index defined as half sum of the distances between all the pairs of vertices in a molecular graph.

If $x, y \in V(G)$ then the *distance* $d_G(x, y)$ between x and y is defined as the length of any shortest path in G connecting x and y. For a vertex u of $V(G)$ its

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eccentricity $\varepsilon_G(u)$ is the largest distance between u and any other vertex v of G, $\varepsilon_G(u) = \max_{v\in V(G)} d_G(u,v)$. The maximum eccentricity over all vertices of G is called the *diameter* of G and denoted by $D(G)$. The *eccentric connectivity index* $\xi(G)$ of a graph G is defined as

$$\xi(G) = \sum_{u\in V(G)} d_G(u)\varepsilon_G(u),$$

where $d_G(u)$ denotes the degree of vertex u in G, i. e., the number of its neighbors in G. When the vertex degrees are not taken into account, we obtain the *total eccentricity* of the graph G, $\zeta(G) = \sum_{u\in V(G)} \varepsilon_G(u)$. For k-regular graphs those two quantities are related as $\xi(G) = k\zeta(G)$. We refer the reader to [2, 4, 6, 9, 15] for explicit formulas for the eccentric connectivity index of various families of graphs. A vertex $u \in V(G)$ is *well-connected* if $\varepsilon_G(u) = 1$, i.e., if it is adjacent to all other vertices in G.

The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajstić [8, 7]. They are defined as:

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

Now we define a new version of Zagreb indices as follows:

$$\begin{aligned} M_1^*(G) &= \sum_{uv\in E(G)} [\varepsilon_G(u) + \varepsilon_G(v)], \\ M_1^{**}(G) &= \sum_{v\in V(G)} (\varepsilon_G(v))^2, \\ M_2^*(G) &= \sum_{uv\in E(G)} \varepsilon_G(u)\varepsilon_G(v). \end{aligned}$$

Here, our notation is standard and mainly taken from standard books of graph theory such as, e.g., [14]. All graphs considered in this paper are simple and connected. The aim of this paper is to compute these new topological indices for some graph operations. To do this, we first consider the following examples:

Example 1. Let K_n be the complete graph on n vertices. Then for every $v \in V(K_n)$, $\varepsilon_G(v) = 1$. This implies that $\zeta(K_n) = n$, $M_1^*(K_n) = n(n-1)$, $M_2^*(K_n) = n(n-1)/2$ and $M_1^{**}(K_n) = n$.

Example 2. Let C_n denote the cycle of length n. It is easy to see that for every $v \in V(C_n)$, $\varepsilon_G(v) = \lfloor n/2\rfloor$. Hence, $\zeta(C_n) = n\lfloor \frac{n}{2}\rfloor$, $M_1^*(C_n) = 2n\lfloor n/2\rfloor$ and $M_1^{**}(C_n) = M_2^*(C_n) = n\lfloor n/2\rfloor^2$.

Example 3. Let $S_n = K_{1,n}$ be the star graph with $n+1$ vertices. The central vertex has degree n and eccentricity 1, while the remaining n vertices have degree

1 and eccentricity 2. Hence, $\zeta(S_n) = 2n + 1$, $M_1^*(S_n) = 3n$, $M_2^*(S_n) = 2n$ and $M_1^{**}(S_n) = 4n + 1$.

Example 4. A wheel W_n is a graph of order $n + 1$ which contains a cycle on n vertices and a central vertex connected to each vertex of the cycle. Again, the central vertex has degree n and eccentricity 1, while the peripheral vertices have degree 3 and eccentricity 2. So, $\zeta(W_n) = 2n+1$, $M_1^*(W_n) = 7n$, $M_2^*(W_n) = 6n$ and $M_1^{**}(W_n) = 4n + 1$.

Example 5. Let P_n be the path on $n \geq 3$ vertices. Then

$$\zeta(P_n) = \begin{cases} n(3n-2)/4 & 2|n \\ (n-1)(3n+1)/4 & 2 \not| n \end{cases},$$

$$M_1^*(P_n) = \begin{cases} (3n^2-6n+4)/2 & 2|n \\ 3(n-1)^2/2 & 2 \not| n \end{cases},$$

$$M_2^*(P_n) = \begin{cases} n(n-2)(7n-10)/12 + n^2/4 & 2|n \\ (n-1)(7n^2-14n+3)/12 & 2 \not| n \end{cases},$$

$$M_1^{**}(P_n) = \begin{cases} n(n-1)(7n-2)/12 & 2|n \\ (n-1)(7n^2-2n-3)/12 & 2 \not| n \end{cases}.$$

2 Main Results

In this section we define some graph operations [10] and then we compute the Zagreb indices for them.

Cartesian product

The *Cartesian product* of two graphs G_1 and G_2 is denoted by $G_1 \square G_2$ has the vertex set $V(G_1) \times V(G_2)$ and, two vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ are connected by an edge if and only if either $([u_1 = v_1$ and $u_2v_2 \in E(G_2)])$ or $([u_2 = v_2$ and $u_1v_1 \in E(G_1)])$. In other word, $|E(G_1 \square G_2)| = |E(G_1)||V(G_2)| + |E(G_2)||V(G_1)|$. The degree of a vertex (u_1, u_2) of $G_1 \square G_2$ is as follows:

$$d_{G_1 \square G_2}(u_1, u_2) = d_{G_1}(u_1) + d_{G_2}(u_2).$$

Lemma 6. $\varepsilon_{G_1 \square G_2}(u_1, u_2) = \varepsilon_{G_1}(u_1) + \varepsilon_{G_2}(u_2)$.

Proof. It is clear that the eccentricity of a vertex $(u_1, u_2) \in V(G_1 \Box G_2)$ cannot exceed the sum of the eccentricities of its projections u_1 and u_2. On the other hand, this upper bound is attained for (w_1, w_2), where w_i is the vertex on which $\varepsilon(u_i)$ is attained, for $i = 1, 2$. This proves the claim. □

The Cartesian product of more than two graphs is denoted by $\prod_{i=1}^{s} G_i$, in which $\prod_{i=1}^{s} G_i = G_1 \Box \ldots \Box G_s = (G_1 \Box \ldots \Box G_{s-1}) \Box G_s$. If $G_1 = G_2 = ... = G_s = G$, we have the s-th Cartesian power of G and denote it by G^s.

Lemma 7. $\varepsilon_{\Box_{i=1}^{k} G_i}((u_1, \cdots, u_k)) = \sum_{i=1}^{k} \varepsilon_{G_i}(u_i)$.

Theorem 8.

$$\begin{aligned}
M_2^*(\Box_{k=1}^{n} G_i) &= \sum_{k=1}^{n} M_1^*(G_k) \sum_{i=1, i\neq k}^{n} \prod_{j=1, j\neq i,k}^{n} |V(G_j)| \zeta(G_i) \\
&+ \sum_{k=1}^{n} |E(G_k)| \sum_{i=1, i\neq k}^{n} \prod_{j=1, j\neq i,k}^{n} |V(G_j)| M_1^{**}(G_i) \\
&+ \sum_{k=1}^{n} M_2^*(G_k) \prod_{i=1, i\neq k}^{n} |V(G_i)| \\
&+ 2\sum_{k=1}^{n} |E(G_k)| \sum_{1\leq i<j\leq n}^{i,j\neq k} \prod_{r=1, r\neq i,j,k}^{n} |V(G_r)| \zeta(G_i)\zeta(G_j).
\end{aligned}$$

Proof. Let $a = (a_1, \cdots, a_k)$ and $b = (b_1, \cdots, b_k)$. Then we have

$$\begin{aligned}
M_2^*(\Box_{k=1}^{n} G_i) &= \sum_{ab\in E(\Box_{k=1}^{n} G_i)} \varepsilon_{\Box_{k=1}^{n} G_i}(a) \varepsilon_{\Box_{k=1}^{n} G_i}(b) \\
&= \sum_{k=1}^{n} \Big(\sum_{a_1\in V(G_1)} \cdots \sum_{a_k b_k \in E(G_k)} \cdots \sum_{a_n \in V(G_n)} \Big(\Big(\varepsilon_{G_k}(a_k) \\
&+ \varepsilon_{G_k}(b_k) \Big) \sum_{i=1, i\neq k}^{n} \Big(\varepsilon_{G_i}(a_i) \Big) + \sum_{i=1, i\neq k}^{n} (\varepsilon_{G_i}(a_i))^2 \Big) \Big) \\
&+ \sum_{k=1}^{n} \Big(\sum_{a_1\in V(G_1)} \cdots \sum_{a_k b_k \in E(G_k)} \cdots \sum_{a_n \in V(G_n)} \Big(\Big(\varepsilon_{G_k}(a_k) \varepsilon_{G_k}(b_k) \\
&+ 2 \sum_{1\leq i<j\leq n}^{i,j\neq k} \varepsilon_{G_i}(a_i) \varepsilon_{G_j}(b_j) \Big) \Big) \Big).
\end{aligned}$$

□

Corollary 9. *Let G and H be graphs. Then*

$$\begin{aligned} M_2^*(G\Box H) &= M_1^*(G)\zeta(H) + M_1^*(H)\zeta(G) + |V(H)|M_1^{**}(G) + |V(G)|M_1^{**}(H) \\ &+ |V(H)|M_2^*(G) + |V(G)|M_1^{**}(H). \end{aligned}$$

Example 10. A Hamming graph $H_{n_1,n_2,\cdots,n_s}$ is defined as $H_{n_1,n_2,\cdots,n_s} = \Box_{i=1}^s K_{n_i}$. So, $M_2^*(H_{n_1,n_2,\cdots,n_s}) = \sum_{k=1}^{s} s^2 \binom{n_k}{2} \prod_{i=1,i\neq k}^{s} n_i$. For $n_1 = n_2 \cdots = n_s = 2$, we achieve the s-dimensional hypercubes Q_s and so, $M_2^*(Q_s) = s^3 2^{s-1}$.

Example 11. Nanotubes and nanotori covered by C_4 are arisen as Cartesian product of a path and a cycle, two cycles, respectively. By Combining examples 2 and 5 with Corollary 9 we obtain the following explicit formulas for nanotubes and nanotori. We denote $R = P_n \Box C_m$ and $S = C_k \Box C_m$ and assume $n \geq 3$. Then

$$M_2^*(R) = \begin{cases} (2n-1)m\lfloor m/2\rfloor^2 + (3n^2-4n+2)m\lfloor m/2\rfloor & \\ +nm(7n^2-15n+11)/6 & 2|n \\ (2n-1)m\lfloor m/2\rfloor^2 + (n-1)(3n-1)m\lfloor m/2\rfloor & \\ +nm(n-1)(7n-8)/6 & 2\not|n \end{cases},$$

$M_2^*(S) = 2km\Big(\lfloor m/2\rfloor^2 + \lfloor k/2\rfloor^2 + 2\lfloor m/2\rfloor\lfloor k/2\rfloor\Big).$

Disjunction and Symmetric Difference

The disjunction $G_1 \vee G_2$ 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 to (v_1, v_2) whenever u_1 is adjacent to v_1 in G_1 or u_2 is adjacent to v_2 in G_2. So,

$$|E(G \vee H)| = |E(G)||V(H)|^2 + |E(H)||V(G)|^2 - 2|E(G)||E(H)|.$$

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 to (v_1, v_2) whenever u_1 is adjacent to v_1 in G_1 or u_2 is adjacent to v_2 in G_2, but not both. From definition one can see that

$$|E(G_1 \oplus G_2)| = |E(G_1)||V(G_2)|^2 + |E(G_2)||V(G_1)|^2 - 4|E(G_1)||E(G_2)|.$$

The distance between any two vertices of a disjunction or a symmetric difference cannot exceed 2. If none of the components contains well-connected vertices, the eccentricity of all vertices is constant and equal to 2.

Lemma 12. *Let G_1 and G_2 be two graphs without well-connected vertices. Then* $\varepsilon_{G_1\oplus G_2}((u_1, u_2)) = \varepsilon_{G_1\vee G_2}((u_1, u_2)) = 2$.

Theorem 13. *Let G and H be two graphs without well-connected vertices. Then*

$$M_2^*(G \vee H) = 4\Big(|E(G)||V(H)|^2 + |E(H)||V(G)|^2 - 2|E(G)||E(H)|\Big),$$

$$M_2^*(G \oplus H) = 4\Big(|E(G)||V(H)|^2 + |E(H)||V(G)|^2 - 4|E(G)||E(H)|\Big).$$

Proof.

$$\begin{aligned} M_2^*(G \vee H) &= \sum_{(u_1,u_2)(v_1,v_2)\in E(G\vee H)} \varepsilon_{G\vee H}((u_1,u_2))\varepsilon_{G\vee H}((v_1,v_2)) \\ &= 4\Big(|E(G)||V(H)|^2 + |E(H)||V(G)|^2 - 2|E(G)||E(H)|\Big), \\ M_2^*(G \oplus H) &= \sum_{(u_1,u_2)(v_1,v_2)\in E(G\oplus H)} \varepsilon_{G\oplus H}((u_1,u_2))\varepsilon_{G\oplus H}((v_1,v_2)) \\ &= 4\Big(|E(G)||V(H)|^2 + |E(H)||V(G)|^2 - 4|E(G)||E(H)|\Big). \quad \square \end{aligned}$$

Join

The join $G = G_1 + G_2$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph union $G_1 \cup G_2$ together with all the edges joining V_1 and V_2. The definition generalizes to the case of $s \geq 3$ graphs in a straightforward manner. The following result is a direct consequence of the definition of join.

Lemma 14. *If none of G_i, $i = 1, 2, \cdots, s$ contains well-connected vertices, then for every $u \in V(G_1 + \cdots + G_s)$ we have $\varepsilon_{G_1+\cdots+G_s}(u) = 2$.*

The following formula for the number of edges is verified by induction on s.

Lemma 15.

$$|E(G_1 + \cdots + G_s)| = \sum_{i=1}^{s} |E(G_i)| + \frac{1}{2}\sum_{i=1}^{s} |V(G_i)| \sum_{j=1, j\neq i}^{s} |V(G_j)|.$$

Theorem 16. *Let $G_i(i = 1, \cdots, s)$ be graphs without well - connected vertices, then*

$$M_2^*(G_1 + \cdots + G_s) = 4|E(G_1 + \cdots + G_s)|.$$

Proof. By using Lemma 15 the proof is clear. $\square$

Composition

The composition $G = G_1[G_2]$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph with vertex set $V(G_1) \times V(G_2)$ and $u = (u_1, v_1)$ is adjacent to $v = (u_2, v_2)$ whenever u_1 is adjacent to u_2 or $u_1 = u_2$ and v_1 is adjacent to v_2. So, $|E(G_1[G_2])| = |E(G_1)||V(G_2)|^2 + |E(G_2)||V(G_1)|$. The asymmetric nature of composition is reflected in the fact that the eccentricity of a vertex of $G_1[G_2]$ is mostly inherited from the "scaffold" graph G_1. The situation is particularly simple when G_1 does not contain any well-connected vertices.

Lemma 17. If G_1 does not contain well-connected vertices, then

$$\varepsilon_{G_1[G_2]}((u,v)) = \varepsilon_{G_1}(u).$$

Proof. Let us consider two vertices, (u_1,u_2) and (v_1,v_2) of $G_1[G_2]$. Consider first the case $u_1 \neq u_2$. Since $d_{G_1[G_2]}((u_1,u_2),(v_1,v_2)) = 1$ whenever u_1 is adjacent to v_1 in G_1, it is clear that the distance between any two vertices in $G_1[G_2]$ is the same as the distance between their projections to G_1. Moreover, their distances is at least 2. It remains to consider the case $u_1 = u_2$. If u_2 is not well-connected in G_2, then any other vertex in the same copy of G_2 can still be reached in at most 2 steps. □

Theorem 18. Let G_1 does not contain well-connected vertices, then

$$M_2^*(G_1[G_2]) = |V(G_2)|^2 M_2^*(G_1) + |E(G_2)| M_1^{**}(G_1).$$

Proof.

$$\begin{aligned} M_2^*(G_1[G_2]) &= \sum_{(u_1,u_2)(v_1,v_2)\in E(G_1[G_2])} \varepsilon_{G_1[G_2]}((u_1,u_2))\varepsilon_{G_1[G_2]}((v_1,v_2)) \\ &= \sum_{u_2,v_2\in V(G_2)} \sum_{u_1v_1\in E(G_1)} \varepsilon_{G_1}(u_1)\varepsilon_{G_1}(v_1) \\ &+ \sum_{u_1\in V(G_1)} \sum_{u_2v_2\in E(G_2)} \Big(\varepsilon_{G_1}(u_1)\Big)^2 \\ &= |V(G_2)|^2 M_2^*(G_1) + |E(G_2)| M_1^{**}(G_1). \end{aligned}$$

□

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