Serdica J. Computing **6** (2012), 409–418

Serdica
Journal of Computing

Bulgarian Academy of Sciences
Institute of Mathematics and Informatics

THE WIENER, ECCENTRIC CONNECTIVITY AND ZAGREB INDICES OF THE HIERARCHICAL PRODUCT OF GRAPHS*

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Abstract. Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two graphs having a distinguished or root vertex, labeled 0. The hierarchical product $G_2 \sqcap G_1$ of G_2 and G_1 is a graph with vertex set $V_2 \times V_1$. Two vertices y_2y_1 and x_2x_1 are adjacent if and only if $y_1x_1 \in E_1$ and $y_2 = x_2$; or $y_2x_2 \in E_2$ and $y_1 = x_1 = 0$. In this paper, the Wiener, eccentric connectivity and Zagreb indices of this new operation of graphs are computed. As an application, these topological indices for a class of alkanes are computed.

1. Introduction. Throughout this paper by the word graph we mean a finite, undirected graph without loops or multiple edges. If two vertices a and b are adjacent then we use the notation $a \sim b$. A graph invariant or topological index is any function on a graph that does not depend on a labeling of its vertices.

ACM Computing Classification System (1998): G.2.2, G.2.3.

Key words: Wiener index, eccentric connectivity index, first Zagreb index, first Zagreb co-index.

*The research of this paper is partially supported by the University of Kashan under grant no 159020/12.

The distance between two vertices u and v of a graph G is denoted by $d_G(u,v)$ ($d(u,v)$ for short). It is defined as the number of edges in a minimum path connecting them. A distance-based topological index is one that is related to the above distance function. The first index is the well-known Wiener index [23] defined as the sum of all distances between vertices of a given graph G.

Let G be a connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. For every vertex $u \in V(G)$, the edge connecting u and v is denoted by uv and $deg_G(u)$ denotes the degree of u in G. The diameter of G, $diam_G(G)$, is the maximum possible distance between any two vertices in the graph. We will omit the subscript G when the graph is clear from the context.

The first and second Zagreb indices [12, 13, 19] were originally defined as

$$M_1(G) = \sum_{u \in V(G)} deg(u)^2$$

and

$$M_2(G) = \sum_{uv \in E(G)} deg(u)deg(v),$$

respectively. These topological indices have numerous applications in chemistry and attracted significant attention from mathematicians [11, 16]. The Zagreb indices can be viewed as the contributions of pairs of adjacent vertices to certain degree-weighted generalizations of Wiener polynomials [9]. It turned out that computing such polynomials for certain composite graphs depends on such contributions from pairs of non-adjacent vertices. The first and second Zagreb co-indices were first introduced by Došlić [9]. They are defined as follows:

$$\begin{aligned} \bar{M_1}(G) &= \sum_{uv \notin E(G)} [deg(u) + deg(v)], \\ \bar{M_2}(G) &= \sum_{uv \notin E(G)} [deg(u)deg(v)]. \end{aligned}$$

In [3], the authors considered some mathematical properties of this new graph invariant.

The eccentricity $\varepsilon_G(u)$ is the largest distance between u and any other vertex v of G. We will omit the subscript G when the graph is clear from the context. The eccentric connectivity index of G is defined as $\xi^c(G) = \sum_{u \in V(G)} \varepsilon(u)deg(u)$ [20].

We encourage the reader to consult papers [1, 2, 21] for some applications and [10, 15, 25] for the mathematical properties of this topological index.

In this article we study graph invariants, the first Zagreb index and co-index, Wiener index and eccentric connectivity index under hierarchical product of graphs [4]. One of us (ARA) in some earlier papers considered the same problem for other graph operations, see [3, 14, 16, 17, 18, 24] for details. Throughout this paper our notation is standard. The complete graph and path on n vertices are denoted by K_n and P_n, respectively. For terms and concepts not defined here we refer the reader to any of several standard monographs such as, e.g., [8] or [22].

2. Main Results. In this section exact formulas for some graph invariants under the hierarchical product of graphs are obtained. The hierarchical product is a new graph operation introduced by Barrière et al. [4]. Following Barrière et al. [5], the binary hypertree of dimension m is defined as the hierarchical product of m copies of the complete graph K_2. Since the graphs obtained from the hierarchical product are spanning subgraphs of the corresponding Cartesian products, we obtain that the binary hypertree of dimension m is a spanning subgraph of the hypercube Q_m. Then the authors applied this fact to obtain some nice results on this class of trees. We refer the interested readers to [6, 7] for a generalization of this concept and some other mathematical properties of hierarchical product.

Let G_1 and G_2 be graphs with vertex sets V_1 and V_2, respectively, having a distinguished or root vertex, labeled 0. The hierarchical product $H = G_2 \sqcap G_1$ is the graph with vertices the tuples x_2x_1, $x_i \in V_i$, $i = 1, 2$, and edges defined as follows:

$$x_2x_1 \sim \begin{cases} x_2y_1, & \text{if } y_1x_1 \in E(G_1), \\ y_2x_1, & \text{if } y_2x_2 \in E(G_2) \text{ and } x_1 = 0. \end{cases}$$

Notice that the structure of the obtained product graph H heavily depends on the root vertices of the factors G_1 and G_2.

Theorem 1. *Suppose G_1 and G_2 are connected graphs with vertex sets V_1 and V_2, respectively. Then* $W(G_2 \sqcap G_1) = |V_2|W(G_1) + |V_1|^2W(G_2) + (|V_2|^2 - |V_2|)|V_1|D_{G_1}(0)$*, where $D_{G_1}(0)$ denotes the summation of all distances between 0 and other vertices of G_1.*

P r o o f. Suppose $x = x_2x_1, y = y_2y_1 \in V(G_2 \sqcap G_1)$, where $x_1, y_1 \in V_1$ and $x_2, y_2 \in V_2$. Apply [4, Proposition 2.4], we have:

$$\begin{aligned} W(G_2 \sqcap G_1) &= \sum_{\{x,y\} \in V(G_2 \sqcap G_1)} d_{G_2 \sqcap G_1}(x, y) \\ &= \sum_{\substack{\{x_1,y_1\} \in V_1 \\ x_2,y_2 \in V_2; x_2 = y_2}} d_{G_1}(x_1, y_1) \\ &+ \sum_{\substack{\{x_1,y_1\} \in V_1 \\ x_2,y_2 \in V_2; x_2 \neq y_2}} (d_{G_2}(x_2, y_2) + d_{G_1}(x_1, 0) + d_{G_1}(0, y_1)) \\ &= |V_2|W(G_1) + |V_1|^2 W(G_2) + (|V_2|^2 - |V_2|)|V_1|D_{G_1}(0), \end{aligned}$$

which completes our argument. □

Corollary 2. *Suppose G is a connected graph. Then the Wiener index of $P_n \sqcap G$ and alkanes $P_n \sqcap P_n$ are computed as follows:*

$$\begin{aligned} W(P_n \sqcap G) &= nW(G) + |V(G)|^2 \frac{n(n^2-1)}{6} + (n^2 - n)|V(G)|D_G(0), \\ W(P_n \sqcap P_n) &= (n^3 + n^2)\frac{(n^2-1)}{6} + n^2(n-1)D_G(0). \end{aligned}$$

Theorem 3. *Suppose G_1 and G_2 are connected graphs. Then $\xi^c(G_2 \sqcap G_1) = (\delta_1 + \delta_2)(\varepsilon_2 + \varepsilon_1) + (\delta_1|V(G_1)| + \delta_2)(\zeta(G_2) - \varepsilon_2) + (|V(G_2)| - 1)(\delta_1 + \delta_2)\varepsilon_1 + \delta_1|V(G_2)|D_{G_1}(0) + |V(G_2)|(|V(G_1)| - 1)\delta_1\varepsilon_1 + \delta_1\varepsilon_2(|V(G_1)| - 1)$, where $\zeta(G) = \sum_{v \in V(G)} \varepsilon(v)$ is called the total eccentricity of G.*

P r o o f. Suppose $x = x_2x_1 \in V(G_2 \sqcap G_1)$ and δ_i and ε_i, $i = 1, 2$, are the degree and eccentricity of root vertex of G_i, respectively. Applying [4, Proposition 2.4] and the definition of hierarchical product of graphs, we have:

$$\xi^c(G_2 \sqcap G_1) = \sum_{x \in V(G_2 \sqcap G_1)} \varepsilon_{V(G_2 \sqcap G_1)}(x) deg_{V(G_2 \sqcap G_1)}(x)$$

$$
\begin{aligned}
&= (\delta_1+\delta_2)(\varepsilon_2+\varepsilon_1) + \sum_{x=x_2 0; x_2\in V(G_2)} (\delta_1+\delta_2)(\varepsilon_{G_2}(x_2)+\varepsilon_1)\\
&+ \sum_{\substack{x=x_2x_1\\ x_1\neq 0\in V(G_1); x_2\in V(G_2)}} \delta_1(\varepsilon_{G_2}(x_2)+d_{G_1}(x_1,0)+\varepsilon_1)\\
&= (\delta_1+\delta_2)(\varepsilon_2+\varepsilon_1) + (\delta_1+\delta_2)\sum_{x_2\neq 0\in V(G_2)} \varepsilon_{G_2}(x_2)\\
&+ (|V(G_2)|-1)(\delta_1+\delta_2)\varepsilon_1 + \delta_1(|V(G_1)|-1)\sum_{x_2\neq 0\in V(G_2)} \varepsilon_{G_2}(x_2)\\
&+ \delta_1|V(G_2)|D_{G_1}(0) + |V(G_2)|(|V(G_1)|-1)\delta_1\varepsilon_1 + \delta_1\varepsilon_2(|V(G_1)|-1)\\
&= (\delta_1+\delta_2)(\varepsilon_2+\varepsilon_1) + (\delta_1|V(G_1)|+\delta_2)(\zeta(G_2)-\varepsilon_2)\\
&+ (|V(G_2)|-1)(\delta_1+\delta_2)\varepsilon_1 + \delta_1|V(G_2)|D_{G_1}(0)\\
&+ |V(G_2)|(|V(G_1)|-1)\delta_1\varepsilon_1 + \delta_1\varepsilon_2(|V(G_1)|-1),
\end{aligned}
$$

which completes our argument. □

Corollary 4. *Suppose G_1 is a connected graph, and δ_1 and ε_1 are the degree and eccentricity of the root vertex of G_1, respectively. Then the eccentric connectivity index of $P_n \sqcap G_1$ and alkanes $P_n \sqcap P_n$ are computed as follows:*

1) *If n is even then:*

$$
\begin{aligned}
\xi^c(P_n \sqcap G_1) &= (\delta_1+\delta_{P_n})(\varepsilon_1+\varepsilon_{P_n}) + (\delta_1|V(G_1)|+\delta_{P_n})\left(\frac{3n^2+2n}{4}-\varepsilon_{P_n}\right)\\
&\quad +(n-1)(\delta_1+\delta_{P_n})\varepsilon_1 + n\delta_1 D_{G_1}(0) + n(|V(G_1)|-1)\delta_1\varepsilon_1\\
&\quad +\delta_1\varepsilon_{P_n}(|V(G_1)|-1),\\
\xi^c(P_n \sqcap P_n) &= 4\delta_{P_n}\varepsilon_{P_n} + \delta_{P_n}(n+1)\left(\frac{3n^2+2n}{4}-\varepsilon_{P_n}\right) + 2(n-1)\delta_{P_n}\varepsilon_{P_n}\\
&\quad +n\delta_{P_n}D_{P_n}(0) + n(n-1)\delta_{P_n}\varepsilon_{P_n} + \delta_{P_n}\varepsilon_{P_n}(n-1).
\end{aligned}
$$

2) *If n is odd then:*

$$\begin{aligned}
\xi^c(P_n \sqcap G_1) &= (\delta_1+\delta_{P_n})(\varepsilon_1+\varepsilon_{P_n})+(n-1)(\delta_1+\delta_{P_n})\varepsilon_1+n\delta_1 D_G(0)\\
&\quad +(\delta_1|V(G_1)|+\delta_{P_n})\left(\frac{3}{4}(n^2-1)+\frac{n-1}{2}-\varepsilon_{P_n}\right)\\
&\quad +n(|V(G_1)|-1)\delta_1\varepsilon_1+\delta_1\varepsilon_{P_n}(|V(G_1)|-1),\\
\xi^c(P_n \sqcap P_n) &= \delta_{P_n}(n+1)\left(\frac{3}{4}(n^2-1)+\frac{n-1}{2}-\varepsilon_{P_n}\right)+2(n+1)\delta_{P_n}\varepsilon_{P_n}\\
&\quad +n\delta_{P_n}D_{P_n}(0)+n(n-1)\delta_{P_n}\varepsilon_{P_n}+\delta_{P_n}\varepsilon_{P_n}(n-1).
\end{aligned}$$

In the following theorem, we use the notations given in the proof of Theorem 3.

Theorem 5. *Suppose G_1 and G_2 are connected graphs. Then the first Zagreb index of the hierarchical product is computed as follows:*

$$M_1(G_2 \sqcap G_1) = |V(G_2)||V(G_1)|{\delta_1}^2+|V(G_2)|{\delta_2}^2+2|V(G_2)|\delta_1\delta_2.$$

Proof. Suppose $H = G_2 \sqcap G_1$ and $x = x_2x_1 \in V(H)$. Consider three separate cases for x and apply [4, Equation 5]. If $x = 00$ then $\deg_H(x) = \delta_1+\delta_2$. If $x = x_20$, $x_2 \neq 0$, then there are $|V(G_2)|-1$ choices for the vertex x_2 and $\deg_H(x) = \delta_1+\delta_2$. Finally, if $x = x_2x_1$, $x_1 \neq 0$, then there are $|V(G_1)|-1$ choices for the vertex x_1, $|V(G_2)|$ choices for x_2 and $\deg_H(x) = \delta_1$.

$$\begin{aligned}
M_1(G_2 \sqcap G_1) &= \sum_{v\in V(G_2\sqcap G_1)} deg^2_{G_2\sqcap G_1}(v)\\
&= (|V(G_2)|-1)(\delta_1+\delta_2)^2+|V(G_2)|(|V(G_1)|-1){\delta_1}^2+(\delta_1+\delta_2)^2\\
&= |V(G_2)||V(G_1)|{\delta_1}^2+|V(G_2)|{\delta_2}^2+2|V(G_2)|\delta_1\delta_2,
\end{aligned}$$

which completes our argument. □

Corollary 6. *With the notations of Theorem 3, we have:*

a) $M_1(P_n \sqcap G_1) = n|V(G_1)|{\delta_1}^2+n{\delta_{P_n}}^2+2n\delta_1\delta_{P_n},$

$$
\begin{aligned}
b)\ M_1(P_n \sqcap P_n) &= {\delta_{P_n}}^2(n^2+3n),\\
c)\ \bar{M}_1(G_2 \sqcap G_1) &= 2|E(G_2 \sqcap G_1)|(|V(G_2 \sqcap G_1)|-1) - M_1(G_2 \sqcap G_1)\\
&= 2(|E(G_2)| + |V(G_2)||E(G_1)|)(|V(G_1)||V(G_2)|-1)\\
&\quad -M_1(G_2 \sqcap G_1),\\
d)\ \bar{M}_1(P_n \sqcap G_1) &= 2(n-1+n|E(G_1)|)(|V(G_1)|n-1) - M_1(P_n \sqcap G_1),\\
e)\ \bar{M}_1(P_n \sqcap P_n) &= 2(n-1)^2 - {\delta_{P_n}}^2(n^2+3n),\\
f)\ M_2(P_n \sqcap G_1) &= (n-1)(\delta_1+1)^2 + n(M_2(G_1) + {\delta_1}^2),\\
g)\ M_2(P_n \sqcap P_n) &= (n-1)(\delta_{P_n}+1)^2 + n(4n-8+{\delta_{P_n}}^2),\\
h)\ \bar{M}_2(P_n \sqcap G_1) &= 2(n-1+n|E(G_1)|)^2 - (n-1)(\delta_1+1)^2\\
&\quad -n(M_2(G_1)+{\delta_1}^2) - \frac{1}{2}(n|V(G_1)|{\delta_1}^2 + n{\delta_{P_n}}^2 + 2n\delta_1\delta_{P_n}),\\
i)\ \bar{M}_2(P_n \sqcap P_n) &= 2(n-1+n(n-1))^2 - (n-1)(\delta_{P_n}+1)^2\\
&\quad -n(4n-8+{\delta_{P_n}}^2) - \frac{1}{2}{\delta_{P_n}}^2(n^2+3n).
\end{aligned}
$$

P r o o f. Apply Theorem 5 and [3, Propositions 2 and 4]. □

Acknowledgment. We are very pleased from the referee for his/her comments and helpful remarks.

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Received September 30, 2012
Final Accepted January 25, 2013