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SOME VARIANTS OF THE SZEGED INDEX UNDER ROOTED PRODUCT OF GRAPHS

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Abstract. The Szeged index $Sz(G)$ of a connected graph G is defined as the sum of the terms $n_u(e|G)n_v(e|G)$ over all edges $e = uv$ of G, where $n_u(e|G)$ is the number of vertices of G lying closer to u than to v and $n_v(e|G)$ is the number of vertices of G lying closer to v than to u. In this paper, some variants of the Szeged index such as the edge PI index, edge Szeged index, edge-vertex Szeged index, vertex-edge Szeged index, and revised edge Szeged index are studied under rooted product of graphs. Results are applied to compute these graph invariants for some chemical graphs by specializing components in rooted products.

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Keywords: edge PI index, edge Szeged index, edge-vertex Szeged index, vertex-edge Szeged index, revised edge Szeged index, rooted product of graphs

1. INTRODUCTION

In this paper, we consider connected finite graphs without loops or multiple edges. Let G be such a graph with vertex set $V(G)$ and edge set $E(G)$. We denote by $d(u,v|G)$ the distance between the vertices u and v in G which is the length of any shortest path in G connecting u and v. Let $e = uv$ be the edge of G connecting the vertices u and v. The quantities $n_0(e|G)$, $n_u(e|G)$, and $n_v(e|G)$ are defined to be the number of vertices of G equidistant from u and v, the number of vertices of G whose distance to u is smaller than the distance to v, and the number of vertices of G whose distance to v is smaller than the distance to u, respectively, i.e.,

$$n_0(e|G) = |\{z \in V(G) : d(z,u|G) = d(z,v|G)\}|,$$

$$n_u(e|G) = |\{z \in V(G) : d(z,u|G) < d(z,v|G)\}|,$$

$$n_v(e|G) = |\{z \in V(G) : d(z,v|G) < d(z,u|G)\}|.$$

For an edge $e = uv \in E(G)$ and a vertex $z \in V(G)$, the distance between z and e is defined as $d(z,e|G) = \min\{d(z,u|G), d(z,v|G)\}$. The quantities $m_0(e|G)$, $m_u(e|G)$, and $m_v(e|G)$ are defined to be the number of edges of G equidistant from u and v, the number of edges of G whose distance to u is smaller than the distance

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to v, and the number of edges of G whose distance to v is smaller than the distance to u, respectively, i.e.,

$$m_0(e|G) = |\{f \in E(G) : d(u, f|G) = d(v, f|G)\}|,$$

$$m_u(e|G) = |\{f \in E(G) : d(u, f|G) < d(v, f|G)\}|,$$

$$m_v(e|G) = |\{f \in E(G) : d(v, f|G) < d(u, f|G)\}|.$$

For the vertex $z \in V(G)$, we define

$$m_z(G) = |\{e = uv \in E(G) : d(u,z|G) \neq d(v,z|G)\}|.$$

Chemical graphs, particularly *molecular graphs*, are graph-based descriptions of molecules, with vertices representing the atoms and edges representing the bonds. A numerical invariant associated with a chemical graph is called *topological index* or *graph invariant*. Topological indices are used in theoretical chemistry for the design of chemical compounds with given physicochemical properties or given pharmacologic and biological activities [6, 20]. The *Wiener index* [21], defined as the sum of distances between all pairs of vertices in a chemical graph, is the oldest and the most thoroughly studied topological index from both theoretical and practical point of view. Motivated by the original definition of the Wiener index, the *Szeged index* [11] was introduced in 1994 which coincides with the Wiener index for a tree. It found applications in quantitative structure-property-activity-toxicity modeling [16]. The Szeged index of a graph G is defined as

$$Sz(G) = \sum_{e=uv\in E(G)} n_u(e|G)n_v(e|G).$$

In recent years, some variants of the Szeged index such as the *vertex PI index* [17], *edge PI index* [15], *edge Szeged index* [12], *edge-vertex Szeged index* [18], *vertex-edge Szeged index* [9], *revised Szeged index* [19], and *revised edge Szeged index* [7] have attracted much attention in both chemistry and mathematics. These indices are defined for a graph G as follows:

$$PI_v(G) = \sum_{e=uv\in E(G)} \big[n_u(e|G) + n_v(e|G)\big],$$

$$PI_e(G) = \sum_{e=uv\in E(G)} \big[m_u(e|G) + m_v(e|G)\big],$$

$$Sz_e(G) = \sum_{e=uv\in E(G)} m_u(e|G)m_v(e|G),$$

$$Sz_{ev}(G) = \frac{1}{2}\sum_{e=uv\in E(G)} \big[n_u(e|G)m_v(e|G) + n_v(e|G)m_u(e|G)\big],$$

$$Sz_{ve}(G) = \frac{1}{2} \sum_{e=uv \in E(G)} \big[n_u(e|G) m_u(e|G) + n_v(e|G) m_v(e|G) \big],$$

$$Sz^*(G) = \sum_{e=uv \in E(G)} \Big[n_u(e|G) + \frac{n_0(e|G)}{2} \Big] \Big[n_v(e|G) + \frac{n_0(e|G)}{2} \Big],$$

$$Sz_e^*(G) = \sum_{e=uv \in E(G)} \Big[m_u(e|G) + \frac{m_0(e|G)}{2} \Big] \Big[m_v(e|G) + \frac{m_0(e|G)}{2} \Big].$$

We refer the reader to [1, 10, 14] for more information on these indices.

The *rooted product* $G_1\{G_2\}$ of a graph G_1 and a rooted graph G_2 is the graph obtained by taking one copy of G_1 and $|V(G_1)|$ copies of G_2, and by identifying the root vertex of the i-th copy of G_2 with the i-th vertex of G_1, for $i = 1, 2, ..., |V(G_1)|$.

In this paper, we study the edge PI index, edge Szeged index, edge-vertex Szeged index, vertex-edge Szeged index, and revised edge Szeged index under rooted product of graphs. Results are applied to compute these invariants for some chemical graphs by specializing components in rooted products. For more information on computing topological indices of rooted product see [2–5, 8, 13, 22].

2. Results and discussion

Let G_1 and G_2 be two connected graphs with vertex sets $V(G_1)$ and $V(G_2)$ and edge sets $E(G_1)$ and $E(G_2)$, respectively. In this section, we compute some variants of the Szeged index for rooted product of G_1 and G_2. Throughout this section, the graph G_2 is assumed to be rooted on the vertex $x \in V(G_2)$ and the degree of x in G_2 is denoted by δ. Also, we denote by n_i and m_i, the order and size of the graph G_i, respectively, where $i \in \{1, 2\}$. In addition, for notational convenience, we define

$$\overline{N} = \sum_{\substack{e=uv \in E(G_2), \\ d(u,x|G_2) < d(v,x|G_2)}} n_v(e|G_2), \quad \underline{N} = \sum_{\substack{e=uv \in E(G_2), \\ d(u,x|G_2) < d(v,x|G_2)}} n_u(e|G_2),$$

$$\overline{M} = \sum_{\substack{e=uv \in E(G_2), \\ d(u,x|G_2) < d(v,x|G_2)}} m_v(e|G_2), \quad \underline{M} = \sum_{\substack{e=uv \in E(G_2), \\ d(u,x|G_2) < d(v,x|G_2)}} m_u(e|G_2).$$

Theorem 1. *The edge PI index of the rooted product $G_1\{G_2\}$ is given by*

$$PI_e(G_1\{G_2\}) = PI_e(G_1) + m_2 PI_v(G_1) + n_1 PI_e(G_2) + n_1\big(m_1 + (n_1 - 1)m_2\big) m_x(G_2). \tag{2.1}$$

Proof. From the definition of the edge PI index, we have

$$PI_e(G_1\{G_2\}) = \sum_{e=uv \in E(G_1\{G_2\})} \big[m_u(e|G_1\{G_2\}) + m_v(e|G_1\{G_2\}) \big].$$

We partition the above sum into two sums as follows:

The first sum S_1 consists of contributions to $PI_e(G_1\{G_2\})$ of edges from G_1,

$$S_1 = \sum_{e=uv\in E(G_1)} \big[m_u(e|G_1\{G_2\}) + m_v(e|G_1\{G_2\})\big].$$

By definition of rooted product, we have

$$\begin{aligned} S_1 &= \sum_{e=uv\in E(G_1)} \Big[\big(m_u(e|G_1) + m_2 n_u(e|G_1)\big) + \big(m_v(e|G_1) + m_2 n_v(e|G_1)\big)\Big] \\ &= \sum_{e=uv\in E(G_1)} \big[m_u(e|G_1) + m_v(e|G_1)\big] \\ &\quad + m_2 \sum_{e=uv\in E(G_1)} \big[n_u(e|G_1) + n_v(e|G_1)\big] \\ &= PI_e(G_1) + m_2 PI_v(G_1). \end{aligned}$$

The second sum S_2 consists of contributions to $PI_e(G_1\{G_2\})$ of edges from n_1 copies of G_2,

$$S_2 = n_1 \sum_{e=uv\in E(G_2)} \big[m_u(e|G_1\{G_2\}) + m_v(e|G_1\{G_2\})\big].$$

By definition of rooted product, we have

$$\begin{aligned} S_2 &= n_1 \sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)\neq d(v,x|G_2)}} \big[m_1 + (n_1-1)m_2 + m_u(e|G_2) + m_v(e|G_2)\big] \\ &\quad + n_1 \sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)= d(v,x|G_2)}} \big[m_u(e|G_2) + m_v(e|G_2)\big] \\ &= n_1\Big[\sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)\neq d(v,x|G_2)}} \big[m_u(e|G_2) + m_v(e|G_2)\big] \\ &\quad + \sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)= d(v,x|G_2)}} \big[m_u(e|G_2) + m_v(e|G_2)\big]\Big] \\ &\quad + n_1\big(m_1 + (n_1-1)m_2\big)\,|\{e = uv \in E(G_2) : d(u,x|G_2) \neq d(v,x|G_2)\}| \\ &= n_1 PI_e(G_2) + n_1\big(m_1 + (n_1-1)m_2\big)m_x(G_2). \end{aligned}$$

Eq. (2.1) is obtained by adding the quantities S_1 and S_2. □

Theorem 2. *The edge Szeged index of the rooted product $G_1\{G_2\}$ is given by*

$$\begin{aligned} Sz_e(G_1\{G_2\}) &= Sz_e(G_1) + m_2^2 Sz(G_1) + 2m_2 Sz_{ev}(G_1) + n_1 Sz_e(G_2) \\ &\quad + n_1\big(m_1 + (n_1-1)m_2\big)\overline{M}. \end{aligned} \tag{2.2}$$

Proof. From the definition of the edge Szeged index, we have

$$Sz_e(G_1\{G_2\}) = \sum_{e=uv\in E(G_1\{G_2\})} m_u(e|G_1\{G_2\})m_v(e|G_1\{G_2\}).$$

We partition the above sum into two sums as follows:
The first sum S_1 consists of contributions to $Sz_e(G_1\{G_2\})$ of edges from G_1,

$$S_1 = \sum_{e=uv\in E(G_1)} m_u(e|G_1\{G_2\})m_v(e|G_1\{G_2\}).$$

By definition of rooted product, we have

$$\begin{aligned}
S_1 &= \sum_{e=uv\in E(G_1)} \big[m_u(e|G_1) + m_2 n_u(e|G_1)\big]\big[m_v(e|G_1) + m_2 n_v(e|G_1)\big] \\
&= \sum_{e=uv\in E(G_1)} m_u(e|G_1)m_v(e|G_1) + m_2^2 \sum_{e=uv\in E(G_1)} n_u(e|G_1)n_v(e|G_1) \\
&\quad + m_2 \sum_{e=uv\in E(G_1)} \big[n_u(e|G_1)m_v(e|G_1) + n_v(e|G_1)m_u(e|G_1)\big] \\
&= Sz_e(G_1) + m_2^2 Sz(G_1) + 2m_2 Sz_{ev}(G_1).
\end{aligned}$$

The second sum S_2 consists of contributions to $Sz_e(G_1\{G_2\})$ of edges from n_1 copies of G_2,

$$S_2 = n_1 \sum_{e=uv\in E(G_2)} m_u(e|G_1\{G_2\})m_v(e|G_1\{G_2\}).$$

By definition of rooted product, we have

$$\begin{aligned}
S_2 &= n_1 \sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)<d(v,x|G_2)}} \big[m_1 + (n_1-1)m_2 + m_u(e|G_2)\big]m_v(e|G_2) \\
&\quad + n_1 \sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)=d(v,x|G_2)}} m_u(e|G_2)m_v(e|G_2) \\
&= n_1\Big[\sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)<d(v,x|G_2)}} m_u(e|G_2)m_v(e|G_2) \\
&\quad + \sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)=d(v,x|G_2)}} m_u(e|G_2)m_v(e|G_2)\Big] \\
&\quad + n_1\big(m_1 + (n_1-1)m_2\big) \sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)<d(v,x|G_2)}} m_v(e|G_2) \\
&= n_1 Sz_e(G_2) + n_1\big(m_1 + (n_1-1)m_2\big)\overline{M}.
\end{aligned}$$

Eq. (2.2) is obtained by adding the quantities S_1 and S_2. □

Theorem 3. *The edge-vertex Szeged index of the rooted product* $G_1\{G_2\}$ *is given by*

$$Sz_{ev}(G_1\{G_2\}) = n_2 Sz_{ev}(G_1) + n_2 m_2 Sz(G_1) + n_1 Sz_{ev}(G_2) + \frac{1}{2}n_1 n_2(n_1-1)\overline{M} + \frac{1}{2}n_1\big(m_1 + m_2(n_1-1)\big)\overline{N}. \quad (2.3)$$

Proof. From the definition of the edge-vertex Szeged index, we have

$$Sz_{ev}(G_1\{G_2\}) = \frac{1}{2}\sum_{e=uv\in E(G_1\{G_2\})}\big[n_u(e|G_1\{G_2\})m_v(e|G_1\{G_2\}) + n_v(e|G_1\{G_2\})m_u(e|G_1\{G_2\})\big].$$

We partition the above sum into two sums as follows:
The first sum S_1 consists of contributions to $Sz_{ev}(G_1\{G_2\})$ of edges from G_1,

$$S_1 = \frac{1}{2}\sum_{e=uv\in E(G_1)}\big[n_u(e|G_1\{G_2\})m_v(e|G_1\{G_2\}) + n_v(e|G_1\{G_2\})m_u(e|G_1\{G_2\})\big].$$

By definition of rooted product, we have

$$\begin{aligned} S_1 &= \frac{1}{2}\sum_{e=uv\in E(G_1)}\Big[n_2 n_u(e|G_1)\big[m_v(e|G_1) + m_2 n_v(e|G_1)\big] \\ &\quad + n_2 n_v(e|G_1)\big[m_u(e|G_1) + m_2 n_u(e|G_1)\big]\Big] \\ &= \frac{1}{2}n_2\sum_{e=uv\in E(G_1)}\big[n_u(e|G_1)m_v(e|G_1) + n_v(e|G_1)m_u(e|G_1)\big] \\ &\quad + n_2 m_2\sum_{e=uv\in E(G_1)} n_u(e|G_1)n_v(e|G_1) \\ &= n_2 Sz_{ev}(G_1) + n_2 m_2 Sz(G_1). \end{aligned}$$

The second sum S_2 consists of contributions to $Sz_{ev}(G_1\{G_2\})$ of edges from n_1 copies of G_2,

$$S_2 = \frac{1}{2}n_1\sum_{e=uv\in E(G_2)}\big[n_u(e|G_1\{G_2\})m_v(e|G_1\{G_2\}) + n_v(e|G_1\{G_2\})m_u(e|G_1\{G_2\})\big].$$

By definition of rooted product, we have

$$S_2 = \frac{1}{2}n_1\sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)<d(v,x|G_2)}}\Big[\big[n_u(e|G_2) + n_2(n_1-1)\big]m_v(e|G_2)$$

$$
\begin{aligned}
&+n_v(e|G_2)\big[m_1+m_2(n_1-1)+m_u(e|G_2)\big]\Big]\\
&+\frac{1}{2}n_1 \sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)=d(v,x|G_2)}} \big[n_u(e|G_2)m_v(e|G_2)+n_v(e|G_2)m_u(e|G_2)\big]\\
=&\frac{1}{2}n_1\Big[\sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)<d(v,x|G_2)}} \big[n_u(e|G_2)m_v(e|G_2)+n_v(e|G_2)m_u(e|G_2)\big]\\
&+\sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)=d(v,x|G_2)}} \big[n_u(e|G_2)m_v(e|G_2)+n_v(e|G_2)m_u(e|G_2)\big]\Big]\\
&+\frac{1}{2}n_1n_2(n_1-1)\sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)<d(v,x|G_2)}} m_v(e|G_2)\\
&+\frac{1}{2}n_1\big(m_1+m_2(n_1-1)\big)\sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)<d(v,x|G_2)}} n_v(e|G_2)\\
=&\,n_1Sz_{ev}(G_2)+\frac{1}{2}n_1n_2(n_1-1)\overline{M}+\frac{1}{2}n_1\big(m_1+m_2(n_1-1)\big)\overline{N}.
\end{aligned}
$$

Eq. (2.3) is obtained by adding the quantities S_1 and S_2. □

Let G be a graph with edge set $E(G)$. We define the *second vertex PI index* of G as

$$PI_v^{(2)}(G)=\sum_{e=uv\in E(G)}\big[n_u(e|G)^2+n_v(e|G)^2\big].$$

Theorem 4 ([9]). *Let G be a graph of order n and size m. Then*

$$Sz^*(G)=\frac{mn^2}{4}-\frac{1}{4}PI_v^{(2)}(G)+\frac{1}{2}Sz(G). \tag{2.4}$$

Theorem 5. *The vertex-edge Szeged index of the rooted product $G_1\{G_2\}$ is given by*

$$
\begin{aligned}
Sz_{ve}(G_1\{G_2\})=&\,n_2Sz_{ve}(G_1)+\frac{1}{2}n_2m_2PI_v^{(2)}(G_1)+n_1Sz_{ve}(G_2)\\
&+\frac{1}{2}n_1n_2(n_1-1)\big(m_1+m_2(n_1-1)\big)m_x(G_2)\\
&+\frac{1}{2}n_1\big(m_1+m_2(n_1-1)\big)\underline{N}+\frac{1}{2}n_1n_2(n_1-1)\underline{M}.
\end{aligned}
\tag{2.5}
$$

Proof. From the definition of the vertex-edge Szeged index, we have

$$Sz_{ve}(G_1\{G_2\}) = \frac{1}{2}\sum_{e=uv\in E(G_1\{G_2\})}\Big[n_u(e|G_1\{G_2\})m_u(e|G_1\{G_2\}) + n_v(e|G_1\{G_2\})m_v(e|G_1\{G_2\})\Big].$$

We partition the above sum into two sums as follows:
The first sum S_1 consists of contributions to $Sz_{ve}(G_1\{G_2\})$ of edges from G_1,

$$S_1 = \frac{1}{2}\sum_{e=uv\in E(G_1)}\Big[n_u(e|G_1\{G_2\})m_u(e|G_1\{G_2\}) + n_v(e|G_1\{G_2\})m_v(e|G_1\{G_2\})\Big].$$

By definition of rooted product, we have

$$\begin{aligned} S_1 &= \frac{1}{2}\sum_{e=uv\in E(G_1)}\Big[n_2n_u(e|G_1)\big[m_u(e|G_1) + m_2n_u(e|G_1)\big] \\ &\quad + n_2n_v(e|G_1)\big[m_v(e|G_1) + m_2n_v(e|G_1)\big]\Big] \\ &= \frac{1}{2}n_2\sum_{e=uv\in E(G_1)}\big[n_u(e|G_1)m_u(e|G_1) + n_v(e|G_1)m_v(e|G_1)\big] \\ &\quad + \frac{1}{2}n_2m_2\sum_{e=uv\in E(G_1)}\big[n_u(e|G_1)^2 + n_v(e|G_1)^2\big] \\ &= n_2Sz_{ve}(G_1) + \frac{1}{2}n_2m_2PI_v^{(2)}(G_1). \end{aligned}$$

The second sum S_2 consists of contributions to $Sz_{ve}(G_1\{G_2\})$ of edges from n_1 copies of G_2,

$$S_2 = \frac{1}{2}n_1\sum_{e=uv\in E(G_2)}\Big[n_u(e|G_1\{G_2\})m_u(e|G_1\{G_2\}) + n_v(e|G_1\{G_2\})m_v(e|G_1\{G_2\})\Big].$$

By definition of rooted product, we have

$$\begin{aligned} S_2 &= \frac{1}{2}n_1\sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)<d(v,x|G_2)}}\Big[\big[n_u(e|G_2) + n_2(n_1-1)\big]\big[m_1 + m_2(n_1-1) \\ &\quad + m_u(e|G_2)\big] + n_v(e|G_2)m_v(e|G_2)\Big] \\ &\quad + \frac{1}{2}n_1\sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)=d(v,x|G_2)}}\big[n_u(e|G_2)m_u(e|G_2) + n_v(e|G_2)m_v(e|G_2)\big] \end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{2}n_1\Big[\sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)<d(v,x|G_2)}} \big[n_u(e|G_2)m_u(e|G_2)+n_v(e|G_2)m_v(e|G_2)\big] \\
&\quad + \sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)=d(v,x|G_2)}} \big[n_u(e|G_2)m_u(e|G_2)+n_v(e|G_2)m_v(e|G_2)\big]\Big] \\
&\quad + \frac{1}{2}n_1n_2(n_1-1)\big(m_1+m_2(n_1-1)\big)\Big|\{e=uv\in E(G_2): d(u,x|G_2) \\
&< d(v,x|G_2)\}\Big| + \frac{1}{2}n_1\big(m_1+m_2(n_1-1)\big) \sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)<d(v,x|G_2)}} n_u(e|G_2) \\
&\quad + \frac{1}{2}n_1n_2(n_1-1) \sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)<d(v,x|G_2)}} m_u(e|G_2) \\
&= n_1 Sz_{ve}(G_2) + \frac{1}{2}n_1n_2(n_1-1)\big(m_1+m_2(n_1-1)\big)m_x(G_2) \\
&\quad + \frac{1}{2}n_1\big(m_1+m_2(n_1-1)\big)\underline{N} + \frac{1}{2}n_1n_2(n_1-1)\underline{M}.
\end{aligned}
$$

Eq. (2.5) is obtained by adding the quantities S_1 and S_2. □

Using Eq. (2.4), we can get an alternative formula for the vertex-edge Szeged index of the rooted product of G_1 and G_2.

Corollary 1. *The vertex-edge Szeged index of the rooted product $G_1\{G_2\}$ is given by*

$$
\begin{aligned}
Sz_{ve}(G_1\{G_2\}) &= n_2Sz_{ve}(G_1) + n_2m_2Sz(G_1) - 2n_2m_2Sz^*(G_1) + n_1Sz_{ve}(G_2) \\
&\quad + \frac{1}{2}n_1^2n_2m_1m_2 + \frac{1}{2}n_1n_2(n_1-1)\big(m_1+m_2(n_1-1)\big)m_x(G_2) \\
&\quad + \frac{1}{2}n_1n_2(n_1-1)\underline{M} + \frac{1}{2}n_1\big(m_1+m_2(n_1-1)\big)\underline{N}. \qquad (2.6)
\end{aligned}
$$

Proof. From Eq. (2.4), we get

$$PI_v^{(2)}(G_1) = m_1n_1^2 - 4Sz^*(G_1) + 2Sz(G_1).$$

Eq. (2.6) is obtained by applying the above equation in Eq. (2.5) and simplifying the resulting expression. □

Let G be a graph with edge set $E(G)$. We define the *second edge PI index* of G as

$$PI_e^{(2)}(G) = \sum_{e=uv\in E(G)} \big[m_u(e|G)^2 + m_v(e|G)^2\big].$$

Theorem 6 ([9])**.** *Let G be a graph of size m. Then*

$$Sz_e^*(G) = \frac{m^3}{4} - \frac{1}{4}PI_e^{(2)}(G) + \frac{1}{2}Sz_e(G). \tag{2.7}$$

Lemma 1. *The second edge PI index of $G_1\{G_2\}$ is given by*

$$\begin{aligned} PI_e^{(2)}(G_1\{G_2\}) = {} & PI_e^{(2)}(G_1) + m_2^2 PI_v^{(2)}(G_1) + 4m_2 Sz_{ve}(G_1) \\ & + n_1 PI_e^{(2)}(G_2) + n_1\big(m_1 + (n_1-1)m_2\big)^2 m_x(G_2) \\ & + 2n_1\big(m_1 + (n_1-1)m_2\big)\underline{M}. \end{aligned} \tag{2.8}$$

Proof. From the definition of the second edge PI index, we have

$$PI_e^{(2)}(G_1\{G_2\}) = \sum_{e=uv\in E(G_1\{G_2\})} \big[m_u(e|G_1\{G_2\})^2 + m_v(e|G_1\{G_2\})^2\big].$$

We partition the above sum into two sums as follows:
The first sum S_1 consists of contributions to $PI_e^{(2)}(G_1\{G_2\})$ of edges from G_1,

$$S_1 = \sum_{e=uv\in E(G_1)} \big[m_u(e|G_1\{G_2\})^2 + m_v(e|G_1\{G_2\})^2\big].$$

By definition of rooted product, we have

$$\begin{aligned} S_1 &= \sum_{e=uv\in E(G_1)} \Big[\big(m_u(e|G_1) + m_2 n_u(e|G_1)\big)^2 + \big(m_v(e|G_1) + m_2 n_v(e|G_1)\big)^2\Big] \\ &= \sum_{e=uv\in E(G_1)} \big[m_u(e|G_1)^2 + m_v(e|G_1)^2\big] \\ &\quad + m_2^2 \sum_{e=uv\in E(G_1)} \big[n_u(e|G_1)^2 + n_v(e|G_1)^2\big] \\ &\quad + 2m_2 \sum_{e=uv\in E(G_1)} \big[n_u(e|G_1)m_u(e|G_1) + n_v(e|G_1)m_v(e|G_1)\big] \\ &= PI_e^{(2)}(G_1) + m_2^2 PI_v^{(2)}(G_1) + 4m_2 Sz_{ve}(G_1). \end{aligned}$$

The second sum S_2 consists of contributions to $PI_e^{(2)}(G_1\{G_2\})$ of edges from n_1 copies of G_2,

$$S_2 = n_1 \sum_{e=uv\in E(G_2)} \big[m_u(e|G_1\{G_2\})^2 + m_v(e|G_1\{G_2\})^2\big].$$

By definition of rooted product, we have

$$S_2 = n_1 \sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)<d(v,x|G_2)}} \Big[\big(m_1 + (n_1-1)m_2 + m_u(e|G_2)\big)^2 + m_v(e|G_2)^2\Big]$$

$$+n_1 \sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)=d(v,x|G_2)}} \left[m_u(e|G_2)^2+m_v(e|G_2)^2\right]$$

$$=n_1\Big[\sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)<d(v,x|G_2)}} \left[m_u(e|G_2)^2+m_v(e|G_2)^2\right]$$

$$+ \sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)=d(v,x|G_2)}} \left[m_u(e|G_2)^2+m_v(e|G_2)^2\right]\Big]$$

$$+n_1\big(m_1+(n_1-1)m_2\big)^2\,|\{e=uv\in E(G_2): d(u,x|G_2)<d(v,x|G_2)\}|$$

$$+2n_1\big(m_1+(n_1-1)m_2\big) \sum_{\substack{e=uv\in E(G_2),\\ d(u,x|G_2)<d(v,x|G_2)}} m_u(e|G_2)$$

$$=n_1 PI_e^{(2)}(G_2)+n_1\big(m_1+(n_1-1)m_2\big)^2 m_x(G_2)+2n_1\big(m_1+(n_1-1)m_2\big)\underline{M}.$$

Eq. (2.8) is obtained by adding the quantities S_1 and S_2. □

Theorem 7. *The revised edge Szeged index of the rooted product $G_1\{G_2\}$ is given by*

$$\begin{aligned} Sz_e^*(G_1\{G_2\}) &= Sz_e^*(G_1)+m_2^2 Sz^*(G_1)+m_2\big(Sz_{ev}(G_1)-Sz_{ve}(G_1)\big)\\ &\quad +n_1 Sz_e^*(G_2)+\frac{1}{2}n_1(m_1+(n_1-1)m_2)(\overline{M}-\underline{M})\\ &\quad -\frac{1}{4}n_1\big(m_1+(n_1-1)m_2\big)^2 m_x(G_2)\\ &\quad +\frac{1}{4}n_1m_2\big[m_1(3m_1+2n_1m_2)+m_2^2(n_1^2-1)\big]. \end{aligned} \tag{2.9}$$

Proof. By Eq. (2.7),

$$Sz_e^*(G_1\{G_2\})=\frac{1}{4}(m_1+n_1m_2)^3-\frac{1}{4}PI_e^{(2)}(G_1\{G_2\})+\frac{1}{2}Sz_e(G_1\{G_2\}).$$

Now using Eq. (2.2) and Eq. (2.8), we get

$$\begin{aligned} Sz_e^*(G_1\{G_2\}) &= \frac{1}{4}\big[m_1^3+3m_1^2n_1m_2+3m_1n_1^2m_2^2+n_1^3m_2^3\big]-\frac{1}{4}\big[PI_e^{(2)}(G_1)\\ &\quad +m_2^2PI_v^{(2)}(G_1)+4m_2Sz_{ve}(G_1)+n_1PI_e^{(2)}(G_2)\\ &\quad +n_1\big(m_1+(n_1-1)m_2\big)^2 m_x(G_2)+2n_1\big(m_1+(n_1-1)m_2\big)\underline{M}\big]\\ &\quad +\frac{1}{2}\big[Sz_e(G_1)+m_2^2Sz(G_1)+2m_2Sz_{ev}(G_1)+n_1Sz_e(G_2)\\ &\quad +n_1\big(m_1+(n_1-1)m_2\big)\overline{M}\big]. \end{aligned}$$

Eq. (2.9) is obtained by simplifying the above expression. □

3. Examples and corollaries

In this section, we apply the results of the previous section to compute the edge PI index, edge Szeged index, edge-vertex Szeged index, vertex-edge Szeged index, and revised edge Szeged index of some graphs by specializing components in rooted product.

Let P_n, S_n, and C_n denote the n-vertex path, star, and cycle, respectively. Some Szeged-related topological indices of these graphs have been given in Table 1.

$Graph$	P_n	S_n	C_n, n is even	C_n, n is odd
PI_v	$n(n-1)$	$n(n-1)$	n^2	$n(n-1)$
PI_e	$(n-1)(n-2)$	$(n-1)(n-2)$	$n(n-2)$	$n(n-1)$
Sz	$\binom{n+1}{3}$	$(n-1)^2$	$\frac{n^3}{4}$	$\frac{n(n-1)^2}{4}$
Sz_e	$\binom{n-1}{3}$	0	$\frac{n(n-2)^2}{4}$	$\frac{n(n-1)^2}{4}$
Sz_{ev}	$\binom{n}{3}$	$\frac{(n-1)(n-2)}{2}$	$\frac{n^2(n-2)}{2}$	$\frac{n(n-1)^2}{2}$
Sz_{ve}	$2\binom{n}{3}$	$\frac{(n-1)^2(n-2)}{2}$	$\frac{n^2(n-2)}{2}$	$\frac{n(n-1)^2}{2}$
Sz^*	$\binom{n+1}{3}$	$(n-1)^2$	$\frac{n^3}{4}$	$\frac{n^3}{4}$
Sz_e^*	$\frac{(n-1)(2n^2-4n+3)}{12}$	$\frac{(n-1)(2n-3)}{4}$	$\frac{n^3}{4}$	$\frac{n^3}{4}$

Table 1. Some topological indices of path, star, and cycle.

As the first example, consider the rooted product of P_n and P_m, where the root vertex of P_m is assumed to be on one of its pendant vertices (vertices of degree one). This molecular graph is called the *comb lattice graph*. Using Eqs. (2.1)–(2.3), (2.6), (2.9), and Table 1, we easily arrive at:

Corollary 2. *Let $G = P_n\{P_m\}$, where the root vertex of P_m is assumed to be on one of its pendant vertices. Then*

(i) $PI_e(G) = (nm-1)(nm-2)$,

(ii) $Sz_e(G) = \frac{nm^3}{6}(3n-2) + \frac{nm^2}{6}(n^2-9n+2) + \frac{11nm}{6} - 1$,

(iii) $Sz_{ev}(G) = \frac{nm^3}{6}(3n-2) + \frac{nm^2}{6}(n^2-6n+2) + \frac{nm}{3}$,

(iv) $Sz_{ve}(G) = \frac{nm^3}{6}(3n^2-3n+2) - \frac{nm^2}{6}(n+1)(n+2) + \frac{2nm}{3}$,

(v) $Sz_e^*(G) = \frac{nm^3}{6}(3n-2) + \frac{nm^2}{6}(n^2-6n+2) + \frac{7nm}{12} - \frac{1}{4}$.

Let $P_n^*(m)$ denote the $m-$*thorn path* which is the graph obtained by attaching m pendant vertices to each vertex of the path P_n. This graph can be viewed as the rooted product of P_n and the star graph on $m+1$ vertices, where the root vertex of S_{m+1} is assumed to be on its central vertex (vertex of degree m). Using Eqs. (2.1)–(2.3), (2.6), (2.9), and Table 1, we easily arrive at:

Corollary 3. *The following equalities hold:*

(i) $PI_e(P_n^*(m)) = n^2m^2 + nm(2n-3) + (n-1)(n-2)$,

(ii) $Sz_e(P_n^*(m)) = \frac{nm^2}{6}(n-1)(n+1) + \frac{nm}{3}(n-1)(n-2) + \binom{n-1}{3}$,

(iii) $Sz_{ev}(P_n^*(m)) = \frac{nm^2}{6}(n^2+3n-1) + \frac{nm}{6}(2n^2-5) + \binom{n}{3}$,

(iv) $$Sz_{ve}(P_n^*(m)) = \frac{n^3m^3}{2} + \frac{nm^2}{6}(8n^2-12n+1) + \frac{nm}{6}(n-1)(7n-11) + 2\binom{n}{3},$$

(v) $Sz_e^*(P_n^*(m)) = \frac{nm^2}{6}(n^2+3n-1) + \frac{nm}{12}(4n^2-7) + \frac{n}{12}(2n^2-6n+7) - \frac{1}{4}$.

Let $C_n^*(m)$ denote the $m-$*thorn cycle* which is the graph obtained by attaching m pendant vertices to each vertex of the cycle C_n. This graph can be seen as the rooted product of C_n and the star graph on $m+1$ vertices, where S_{m+1} is assumed to be rooted on its central vertex. Using Eqs. (2.1)–(2.3), (2.6), (2.9), and Table 1, we easily arrive at:

Corollary 4. *The following equalities hold:*

(i) $$PI_e(C_n^*(m)) = \begin{cases} n^2m^2 + nm(2n-1) + n(n-2) & n \text{ is even}, \\ n^2m^2 + 2nm(n-1) + n(n-1) & n \text{ is odd}, \end{cases}$$

(ii) $$Sz_e(C_n^*(m)) = \begin{cases} \frac{n(nm+n-2)^2}{4} & n \text{ is even}, \\ \frac{n(n-1)^2(m+1)^2}{4} & n \text{ is odd}, \end{cases}$$

(iii) $$Sz_{ev}(C_n^*(m)) = \begin{cases} \frac{n^2m^2}{4}(n+2) + \frac{nm}{2}(n^2-1) + \frac{n^2}{4}(n-2) & n \text{ is even}, \\ \frac{nm^2}{4}(n^2+1) + \frac{n^2m}{2}(n-1) + \frac{n(n-1)^2}{4} & n \text{ is odd}, \end{cases}$$

(iv) $$Sz_{ve}(C_n^*(m)) = \begin{cases} \frac{n^3m^3}{2} + \frac{n^2m^2}{4}(5n-4) + \frac{nm}{2}(2n^2-3n+1) + \frac{n^2(n-2)}{4}, & n \text{ is even} \\ \frac{n^3m^3}{2} + \frac{nm^2}{4}(5n^2-6n+1) + nm(n-1)^2 + \frac{n(n-1)^2}{4}, & n \text{ is odd} \end{cases}$$

(v) $Sz_e^*(C_n^*(m)) = \frac{n^2m^2}{4}(n+2) + \frac{nm}{4}(2n^2+2n-1) + \frac{n^3}{4}$.

Finally, consider the rooted product of P_n and C_m. Note that because of the symmetry of C_m any vertex of this graph can be considered at its root vertex. Using Eqs. (2.1)–(2.3), (2.6), (2.9), and Table 1, we easily arrive at:

Corollary 5. *Let $G = P_n\{C_m\}$. Then*

(i) $$PI_e(G) = \begin{cases} n^2m^2 + 2nm(n-2) + (n-1)(n-2) & m \text{ is even}, \\ n^2m^2 + nm(n-2) - 2(n-1) & m \text{ is odd}, \end{cases}$$

(ii) $$Sz_e(G) = \begin{cases} \frac{nm^3}{4}(2n-1) + \frac{nm^2}{6}(n+1)(n-4) & m \text{ is even} \\ +\frac{nm}{3}(n-2)(n-4) + \binom{n-1}{3}, & \\ \frac{nm^3}{4}(2n-1) + \frac{nm^2}{6}(n^2-3n-1) & m \text{ is odd} \\ +\frac{nm}{12}(4n^2-18n+17) + \frac{n-1}{6}(n^2-2n+6), & \end{cases}$$

(iii) $$Sz_{ev}(G) = \begin{cases} \frac{n^2m^3}{2} + \frac{nm^2}{12}(2n^2-3n-11) + m\binom{n}{3} & m \text{ is even}, \\ \frac{n^2m^3}{2} + \frac{nm^2}{12}(2n^2-9n-5) & m \text{ is odd} \\ +\frac{nm}{6}(n^2-3n+5) + \frac{n(n-1)}{4}, & \end{cases}$$

(iv) $$Sz_{ve}(G) = \begin{cases} \frac{nm^3}{2}(n^2-n+1) + \frac{nm^2}{12}(10n^2-21n-1) & m \text{ is even} \\ +2m\binom{n}{3}, & \\ \frac{nm^3}{2}(n^2-n+1) + \frac{nm^2}{12}(4n^2-15n-1) & m \text{ is odd} \\ -\frac{nm}{6}(n^2-4) + \frac{n(n-1)}{4}, & \end{cases}$$

(v) $$Sz_e^*(G) = \begin{cases} \frac{nm^3}{4}(2n-1) + \frac{nm^2}{6}(n-1)(n+4) & m \text{ is even} \\ +\frac{nm}{6}(2n^2-3n+1) + \frac{n-1}{12}(2n^2-4n+3), & \\ \frac{nm^3}{4}(2n-1) + \frac{5m^2}{2}\binom{n+1}{3} + \frac{nm}{6}(5n^2-9n+4) & m \text{ is odd} \\ +\frac{1}{12}(5n^3-12n^2+10n-3). & \end{cases}$$

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