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Revised and edge revised Szeged indices of graphs

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Abstract

The revised Szeged index is a molecular structure descriptor equal to the sum of products $[n_u(e) + n_0(e)/2] \times [n_v(e) + n_0(e)/2]$ over all edges $e = uv$ of the molecular graph G, where $n_0(e)$ is the number of vertices equidistant from u and v, $n_u(e)$ is the number of vertices whose distance to vertex u is smaller than the distance to vertex v and $n_v(e)$ is defined analogously. In this paper, new formula for computing this molecular descriptor is presented by which it is possible to reprove most of results given in [M. Aouchiche and P. Hansen, On a conjecture about the Szeged index, *European J. Combin.* **31** (2010), 1662–1666]. We also present an edge version of this graph invariant. At the end of the paper an open question is presented.

Keywords: Szeged index, edge Szeged index, revised Szeged index, edge revised Szeged index.

Math. Subj. Class.: 05C12

1 Introduction

We first describe some notations which will be kept throughout. Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. If $e = uv \in E(G)$ then $d(u, v)$ stands for the distance between u and v in G. A *topological index* is a graph invariant applicable in chemistry. A topological index χ is called *distanced-based*, if χ is related to the distance function $d(-, -)$. The first use of a distance-based topological index occurred in the year 1947 in a seminal paper by an American chemist Harold Wiener [14].

Suppose G is a connected graph and $e = uv \in E(G)$. The quantities $n_0(e)$, $n_u(e)$ and $n_v(e)$ are defined to be the number of vertices equidistant from u and v, the number of vertices whose distance to vertex u is smaller than the distance to vertex v and the number

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of vertices closer to v than u, respectively. Similarly, the quantities $m_0(e)$, $m_u(e)$ and $m_v(e)$ are defined to be the number of edges equidistant from u and v, the number of edges whose distance to vertex u is smaller than the distance to vertex v and the number of edges closer to v than u, respectively. Here, for an edge $e = xy$ and vertex u, the distance between e and u is defined as $d_G(e, u) = Min\{d_G(x, u), d_G(y, u)\}$.

The *Szeged*, *edge Szeged*, *edge-vertex Szeged*, *vertex-edge Szeged*, *revised Szeged* and *edge revised Szeged* indices of G are defined as follows:

$$\begin{aligned}
Sz(G) &= \sum_{e=uv} [n_u(e) \times n_v(e)], \\
Sz_e(G) &= \sum_{e=uv} [m_u(e) \times m_v(e)], \\
Sz_{ev}(G) &= 1/2 \sum_{e=uv} [m_u(e) \times n_v(e) + m_v(e) \times n_u(e)], \\
Sz_{ve}(G) &= 1/2 \sum_{e=uv} [m_u(e) \times n_u(e) + m_v(e) \times n_v(e)], \\
Sz^*(G) &= \sum_{e=uv} [(n_u(e) + n_0(e)/2) \times (n_v(e) + n_0(e)/2)], \\
Sz_e^*(G) &= \sum_{e=uv} [(m_u(e) + m_0(e)/2) \times (m_v(e) + m_0(e)/2)].
\end{aligned}$$

It is worth mentioning here that the Szeged index was introduced by Ivan Gutman [4] and the name Szeged index was given in [5]. For the mathematical properties of this topological index we refer to [3, 9, 10]. The concept of edge Szeged index was introduced in [6] and mathematical properties of this graph invariant are studied in [2, 7, 8]. The revised Szeged index was introduced by Milan Randić [13] as a modification of the classical Wiener index. Nowadays the scientists prefer the name revised Szeged index for this distance-based topological index. The interested readers can consult [1, 11, 12, 15] for mathematical properties of this new topological index.

Throughout this section graph means finite simple connected graph. The notation is standard and can be taken from the standard books on graph theory.

2 Main results

In this section, we first present a new formula for computing revised Szeged index of graphs. Then apply this new formula to reprove all results given by Aouchiche and Hansen [1]. We also present an edge version of the revised Szeged index and extend the results given in the mentioned article to this new graph invariant. We begin by an example.

Example 2.1. Suppose $G_1 = K_n$, $G_2 = C_n$ and $G_3 = W_n$ denote the complete, cycle and wheel graphs of order n, and $G_4 = K_{m,n}$ is the complete bipartite graph with partitions of size m and n, respectively. Then,

- If $e = uv \in E(G_1)$ then $m_u = m_v = n - 2$ and $m_0 = \frac{n^2-5n+8}{2}$. Therefore, $Sz_e(G_1) = \frac{n(n-1)(n-2)^2}{2}$ and $Sz_e^*(G_1) = \frac{n^3(n-1)^3}{32}$.
- Suppose $e = uv$ is an arbitrary edge of G_2. If $n = 2k + 1$, then $m_u = m_v = k$ and so $m_0 = 1$. Therefore, $Sz_e(G_2) = (2k + 1)k^2 = \frac{n(n-1)^2}{4}$ and $Sz_e^*(G_2) = \frac{n^3}{4}$.

If $n = 2k$ then $m_u = m_v = k-1$ and so $m_0 = 2$. This implies that $Sz_e(G_2) = n(k-1)^2 = \frac{n(n-2)^2}{4}$ and $Sz_e^*(G_2) = \frac{n^3}{4}$.

- Consider the $n-$vertex wheel graph G_3, $n > 5$. If $e = uv$ is an edge of G_3 such that the vertex v is the center of G_3, then $m_u = 3$, $m_v = 2n-7$ and $m_0 = 3$. If both of u and v are not the center of G_3, then $m_u = 3$, $m_v = 3$ and $m_0 = 2n-8$. Therefore $Sz_e(G_3) = (n-1)(4n-5)$ and $Sz_e^*(G_3) = (n-1)(n^2+5n-73/4)$.
- Suppose $G_4 = K_{x,y}$, $x+y = n$, is the complete bipartite graph containing an arbitrary edge $e = uv$, where $deg(u) = x$ and $deg(v) = y$. Then we have $m_u = x-1, m_v = y-1, m_0 = xy-x-y+2$. This implies that $Sz_e(G_4) = xy(x-1)(y-1)$ and $Sz_e^*(G_4) = \frac{xy}{4}(x^2y^2 - x^2 - y^2 + 2xy)$.

Theorem 2.2. *Let G be an n-vertex and m-edge graph. Then*

$$Sz^*(G) = \frac{mn^2}{4} - \frac{1}{4}\sum_{e=uv}(n_u^2 + n_v^2) + \frac{1}{2}Sz(G)$$

Proof. Since $n_u(e) + n_v(e) = n - n_0(e)$ we have:

$$\begin{aligned}
Sz^*(G) &= \sum_{e=uv}\left[(n_u + \frac{n_0}{2})(n_v + \frac{n_0}{2})\right] \\
&= \sum_{e=uv}\left[n_u n_v + \frac{n_0}{2}(n_u+n_v) + \frac{1}{4}n_0^2\right] \\
&= \sum_{e=uv}\left[n_u n_v + \frac{1}{2}((n-(n_u+n_v)))(n_u+n_v) + \frac{1}{4}(n-(n_u+n_v))^2\right] \\
&= \sum_{e=uv}\left[n_u n_v + \frac{n}{2}(n_u+n_v) - \frac{1}{2}(n_u+n_v)^2\right. \\
&\qquad \left. + \ \frac{n^2}{4} - \frac{1}{2}n(n_u+n_v) + \frac{1}{4}(n_u+n_v)^2\right] \\
&= \sum_{e=uv}\left[n_u n_v + \frac{n^2}{4} - \frac{1}{4}(n_u^2 + n_v^2 + 2(n_u)(n_v))\right] \\
&= \frac{1}{2}Sz(G) + \frac{mn^2}{4} - \frac{1}{4}\sum_{e=uv}[n_u^2 + n_v^2].
\end{aligned}$$

proving the result. □

The next Corollary is already known result that stated and proven in [1].

Corollary 2.3. $Sz(G) \le Sz^*(G) \le \frac{mn^2}{4}$.

Proof. Since $n_u + n_v \le n$, $(n_u+n_v)^2 \le n^2$. So, $\sum_{e=uv}[n_u+n_v]^2 \le mn^2$ and therefore $\frac{mn^2}{4} - \frac{1}{4}\sum_{e=uv}[n_u+n_v]^2 = \frac{mn^2}{4} - \frac{1}{4}\sum_{e=uv}[n_u^2+n_v^2] - \frac{1}{2}Sz(G) \ge 0$. Now, Theorem 2.2 implies that $Sz(G) \le Sz^*(G)$, the left hand side of inequality. The right hand side is a direct consequence of Theorem 2.2 and the following inequality:

$$\frac{1}{2}Sz(G) - \frac{1}{4}\sum_{e=uv}[n_u^2 + n_v^2] = -\frac{1}{4}\sum_{e=uv}[n_u - n_v]^2 \le 0.$$

□

By a similar argument as Theorem 2.2, one can prove:

Theorem 2.4. *Let G be an n-vertex and m-edge graph. Then*

$$Sz_e^*(G) = \frac{m^3}{4} - \frac{1}{4}\sum_{e=uv}[m_u^2 + m_v^2] + \frac{1}{2}Sz_e(G).$$

Corollary 2.5. $Sz_e(G) \leq Sz_e^*(G) \leq \frac{m^3}{4}$.

Proof. The proof is similar to the proof of Corollary 2.3 and so omitted. □

Suppose G is a connected graph and u is a vertex of G. Define

$$D(u,G) = \sum_{x\in V(G)}[d_G(u,x)].$$

The graph G is called *distance-balanced* (or *transmission-regular* according to [1]) if for every $u, v \in V(G)$, $D(u,G) = D(v,G)$. Similarly for a vertex u and an edge $e = xy$ define $D_e(u,G) = \sum_{e\in E(G)}[d_G(e,u)$. A graph G is called *edge-distance-balanced* if for every vertices $u, v \in V(G)$, $D_e(u,G) = d_e(v,G)$.

Theorem 2.6. *Suppose u and v are vertices of a connected graph G. Then $m_u = m_v$ if and only if $D_e(u,G) = d_e(v,G)$.*

Proof. Let $e = uv$ be an arbitrary edge of G. We partition the edge set of G into three parts as follows:

- $M(u)$ is the set of all edges that are closer to u than v.
- $M(v)$ is the set of all edges that are closer to v than u.
- $M(o)$ is the set of all edges that are equidistant from u and v.

Suppose $m_u(e) = |M(u)|$, $m_v(e) = |M(v)|$ and $m_0(e) = |M(o)|$. Then we have :

$$\begin{aligned}
D_e(u,G) &= \sum_{e\in E(G)} d_G(e,u)\\
&= \sum_{e\in M(u)} d_G(e,u) + \sum_{e\in M(v)} d_G(e,u) + \sum_{e\in M(0)} d_G(e,u)\\
&= \sum_{e\in M(u)} d_G(e,u) + \sum_{e\in M(v)} (1 + d_G(e,v)) + \sum_{e\in M(0)} d_G(e,u)\\
&= \sum_{e\in M(u)} d_G(e,u) + m_v(e) + \sum_{e\in M(v)} d_G(e,v) + \sum_{e\in M(0)} d_G(e,u).
\end{aligned}$$

A similar argument shows that

$$D_e(v,G) = \sum_{e\in M(u)} d_G(e,u) + m_u(e) + \sum_{e\in M(v)} d_G(e,v) + \sum_{e\in M(0)} d_G(e,v).$$

But $D_e(u,G) - D_e(v,G) = m_v(e) - m_u(e)$ and so $m_u(e) = m_v(e)$ if and only if $D_e(u,G) = D_e(v,G)$. This complete our argument. □

Corollary 2.7. *If $Sz_e(G) = \frac{m^3}{4}$ then G is an edge-distance-balanced graph.*

Proof. If $Sz_e(G) = \frac{m^3}{4}$ then by Corollary 2.5, $Sz_e^*(G) = \frac{m^3}{4}$. Thus

$$\frac{1}{2}Sz_e(G) - \frac{1}{4}\sum_{uv\in E(G)}[m_u^2 + m_v^2] = -\frac{1}{4}\sum_{uv\in E(G)}[m_u - m_v]^2 = 0.$$

Therefore $m_u = m_v$. Now Theorem 2.6 implies that G is an edge-distanced-balanced graph. □

In the end of this paper, we compute an exact formula for the edge revised Szeged index of Cartesian product of graphs. To do this, we assume that G and H are connected graphs with vertex sets $V(G) = \{u_1, u_2, ..., u_r\}$ and $V(H) = \{v_1, v_2, \dots, v_s\}$. We also assume that $|E(G)| = e_1$ and $|E(H)| = e_2$. Then by definition $V(G \times H) = V(G) \times V(H)$ and we have:

$$E(G \times H) = \{(u, v)(a, b) \mid [u = a, vb \in E(H)] \text{ or } [ua \in E(G), v = b]\}.$$

Clearly, $|E(G \times H)| = |V(G)||E(H)| + |V(H)||E(G)|$. To compute the edge revised Szeged index of $G \times H$ we partition the edge set of this graph into the following parts:

$$\begin{aligned} A_m &= \{(u_m, x)(u_m, y) \mid xy \in E(H)\}\ ;\ 1 \leq m \leq r, \\ B_t &= \{(a, v_t)(b, v_t) \mid ab \in E(G)\}\ ;\ 1 \leq t \leq s. \end{aligned}$$

Theorem 2.8. *(See [15, Lemmas 2 and 3]). With above notations we have:*
(a) If $e = (u_m, v_j)(u_m, v_q) \in A_m$) then

$$\begin{aligned} m_{(u_m,v_j)}(e) &= |V(G)|m_{v_j}(v_jv_q) + |E(G)|n_{v_j}(v_jv_q) = rm_{v_j}(H) + e_1n_{v_j}(H), \\ m_{(u_m,v_q)}(e) &= |V(G)|m_{v_q}(v_jv_q) + |E(G)|n_{v_j}(v_jv_q) = rm_{v_q}(H) + e_1n_{v_q}(H). \end{aligned}$$

(b) If $e = (u_i, v_t)(u_p, v_t) \in B_t$ then

$$\begin{aligned} m_{(u_i,v_t)}(e) &= |V(H)|m_{u_i}(u_iu_p) + |E(H)|n_{u_i}(u_iu_p) = sm_{u_i}(G) + e_2n_{u_i}(G), \\ m_{(u_p,v_t)}(e) &= |V(H)|m_{u_p}(u_iu_p) + |E(H)|n_{u_p}(u_iu_p) = sm_{u_p}(G) + e_2n_{u_p}(G). \end{aligned}$$

Theorem 2.9. *With notation of Theorem 2.8, the edge revised Szeged index of Cartesian product of G and H can be computed as follows:*

$$\begin{aligned} Sz_e^*(G \times H) &= \frac{1}{2}r^3Sz_e(H) + r^2e_1Sz_{ev}(H) + \frac{1}{2}re_1^2Sz(H) + \frac{1}{4}re_2(re_2 + se_1)^2 \\ &- r^2e_1Sz_{ve}(H) - \frac{1}{4}r^3\sum_{xy\in E(H)}[m_x^2(H) + m_y^2(H)] \\ &- \frac{1}{4}re_1^2\sum_{xy\in E(H)}[n_x^2(H) + n_y^2(H)] + \frac{1}{2}s^3Sz_e(G) + s^2e_2Sz_{ev}(G) \\ &+ \frac{1}{2}se_2^2Sz(G) + \frac{1}{4}se_1(se_1 + re_2)^2 - s^2e_2Sz_{ve}(G) \\ &- \frac{1}{4}s^3\sum_{ab\in E(G)}[m_a^2(G) + m_b^2(G)] - \frac{1}{4}se_2^2\sum_{ab\in E(G)}[n_a^2(G) + n_b^2(G)]. \end{aligned}$$

Proof. Let $e = (u_m, x)(u_m, y) \in A_m$. Then $m_0(e) = re_2 + se_1 - r(m_x(H) + m_y(H)) - e_1(n_x(H) + n_y(H))$. Set,

$$\begin{aligned} A &= \left[m_{(u_m,x)}(e) + \frac{m_0(e)}{2}\right] \times \left[m_{(u_m,y)}(e) + \frac{m_0(e)}{2}\right], \\ B &= \left[m_{(a,v_t)}(e) + \frac{m_0(e)}{2}\right] \times \left[m_{(b,v_t)}(e) + \frac{m_0(e)}{2}\right]. \end{aligned}$$

Then we have:

$$\begin{aligned} A &= \frac{1}{2}r^2 m_x(H)m_y(H) + \frac{1}{2}e_1 r(n_x(H)m_y(H) + n_y(H)m_x(H)) \\ &+ \frac{1}{2}e_1^2 n_x(H)n_y(H) + \frac{1}{4}(re_2 + se_1)^2 - \frac{1}{2}e_1 r(n_x(H)m_x(H) + n_y(H)m_y(H)) \\ &- \frac{1}{4}r^2(m_x^2(H) + m^2y(H)) - \frac{1}{4}e_1^2(n_x^2(H) + n_y^2(H)). \end{aligned}$$

Thus,

$$\begin{aligned} \sum_{(u_m,x)(u_m,y)\in A_m} & \left[m_{(u_m,x)}(e) + \frac{m_o(e)}{2}\right]\left[m_{(u_m,y)}(e) + \frac{m_0(e)}{2}\right] \\ &= 1/2r^2 Sz_e(H) + e_1 r Sz_{ev}(H) + \frac{1}{2}e_1^2 Sz(H) + \frac{1}{4}e_2(re_2 + se_1)^2 \\ &- e_1 r Sz_{ve}(H) - \frac{1}{4}r^2 \sum_{xy\in E(H)} [m_x^2(H) + m_y^2(H)] \qquad (2.1) \\ &- \frac{1}{4}e_1^2 \sum_{xy\in E(H)} [n_x^2(H) + n_y^2(H)]. \end{aligned}$$

Using a similar argument for the edge $e = (a, v_t)(b, v_t) \in B_t$, we have:

$$\begin{aligned} B &= \left[m_{(a,v_t)}(e) + \frac{m_0(e)}{2}\right]\left[m_{(b,v_t)}(e) + \frac{m_0(e)}{2}\right] \\ &= \frac{1}{2}s^2 m_{u_i}(G)m_{u_p}(G) + \frac{1}{2}e_2 s\left[n_a(G)m_b(G) + n_b(G)m_a(G)\right] \\ &+ \frac{1}{2}e_2^2 n_a(G)n_b(G) + \frac{1}{4}(se_1 + re_2)^2 - \frac{1}{2}e_2 s\left[n_a(G)m_a(G) + n_b(G)m_b(G)\right] \\ &- \frac{1}{4}s^2\left[m_a^2(G) + m_b^2(G)\right] - \frac{1}{4}e_2^2\left[n_a^2(G) + n_b^2(G)\right]. \end{aligned}$$

So,

$$\begin{aligned} \sum_{(a,v_t)(b,v_t)\in B_t} & \left[m_{(a,v_t)}(e) + \frac{m_0(e)}{2}\right]\left[m_{(b,v_t)}(e) + \frac{m_0(e)}{2}\right] \\ &= \frac{1}{2}s^2 Sz_e(G) + e_2 s Sz_{ev}(G) + \frac{1}{2}e_2^2 Sz(G) + \frac{1}{4}e_1(se_1 + re_2)^2 \\ &- e_2 s Sz_{ve}(G) - \frac{1}{4}s^2 \sum_{ab\in E(G)} \left[m_a^2(G) + m_b^2(G)\right] \qquad (2.2) \\ &- \frac{1}{4}e_2^2 \sum_{ab\in E(G)} \left[n_a^2(G) + n_b^2(G)\right]. \end{aligned}$$

Now multiplying Eq. (2.1) by r and Eq. (2.2) by s and summation of these values, the formula given in the theorem will be obtained. □

3 Conclusions

Some of mathematicians recently focus on the revised Szeged index of graphs. In this paper a new formula for computing this topological index is presented by which it is possible to reprove some earlier results. We also investigate an edge version of this interesting topological index. We proved that the edge version of this graph invariant is more complicated than its vertex version. In the case of vertex version, it is easy to find an exact formula for the Cartesian product of graphs but in the edge version it is too difficult.

In Theorem 2.6 and Corollary 2.7, it is proved that $Sz_e(G) = \frac{m^3}{4}$ implies that G is an edge-balanced-distance graph. We end the paper with the following open question:

Question: Characterize graphs G such that $Sz_e(G) = m^3/4$.

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