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SPLICE GRAPHS AND THEIR TOPOLOGICAL INDICES

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ABSTRACT. Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two graphs with disjoint vertex sets V_1 and V_2. Let $u_1 \in V_1$ and $u_2 \in V_2$. A splice of G_1 and G_2 by vertices u_1 and u_2, $\mathcal{S}(G_1, G_2; u_1, u_2)$, is defined by identifying the vertices u_1 and u_2 in the union of G_1 and G_2. In this paper we calculate the Szeged, edge-Szeged, PI, vertex-PI and eccentric connectivity indices of splice graphs.

1 Introduction

Let $G = (V, E)$ be a simple graph with V and E being its vertex and edge sets, respectively. Graph theory has successfully provided chemists with a variety of useful tools [2, 5, 7, 8, 15], among which are the topological indices or molecular–graph–based structure descriptors [11–14, 23, 24]. In this paper we are concerned with five of these topological indices, that recently attracted much attention and found noteworthy chemical applications.

All graphs considered in this paper are assumed to be simple, undirected, without weighted edges, and connected.

The **Szeged index** of a graph G is denoted by $Sz(G)$ and defined as [6]

$$Sz = Sz(G) = \sum_{e=uv} n_u(e)\, n_v(e) \ . \tag{1.1}$$

Here the sum is taken over all edges of G, and for a given edge $e = uv$, the quantity $n_u(e)$ denotes the number of vertices closer to u than to v, and the quantity $n_v(e)$ is defined analogously. For more details on the Szeged index see the review [10] and the references cited therein.

Denote by $d_G(x, y)$ the distance (= number of edges in a shortest path) between the vertices x and y of the graph G. Then we can define the sets

$$N(e, u, G) = \Big\{x \in V(G) \,|\, d_G(x, u) < d_G(x, v)\Big\}$$

and

$$N(e, v, G) = \Big\{x \in V(G) \,|\, d_G(x, v) < d_G(x, u)\Big\}$$

by means of which we have:

$$n_u(e) = n_u(e, G) = \Big|N(e, u, G)\Big| \qquad \text{and} \qquad n_v(e) = n_v(e, G) = \Big|N(e, v, G)\Big| \ .$$

It is obvious that an end-vertex of any edge is closer to itself than to the other end-vertex of that edge. Therefore the product $n_u(e)\, n_v(e)$ is always positive.

The **edge-Szeged index** is obtained by replacing $n_u(e)\, n_v(e)$ in Eq. (1.1) by $m_u(e)\, m_v(e)$, where $m_u(e)$ is the number of edges in G whose distance to vertex u is smaller than the distance to vertex v, and $m_v(e)$ is defined analogously. Hence the edge version of the Szeged index is given by [9]

$$Sz_e = Sz_e(G) = \sum_{e=uv} m_u(e)\, m_v(e) \ .$$

We recall that the distance between the edge $f = xy$ and the vertex u in the graph G, denoted by $d_G(f, u)$, is define as $d_G(f, u) = \min\Big\{d_G(x, u), d_G(y, u)\Big\}$. We can now introduce the sets

$$M(e, u, G) = \Big\{f \in E(G) \,|\, d_G(f, u) < d_G(f, v)\Big\}$$

and

$$M(e, v, G) = \Big\{f \in E(G) \,|\, d_G(f, v) < d_G(f, u)\Big\}$$

by means of which we have:

$$m_u(e) = m_u(e,G) = \Big|M(e,u,G)\Big| \qquad \text{and} \qquad m_v(e) = m_v(e,G) = \Big|M(e,v,G)\Big| \,.$$

If instead of multiplicative contributions $n_u(e)\, n_v(e)$ and $m_u(e)\, m_v(e)$, we consider their additive versions, $n_u(e) + n_v(e)$ and $m_u(e) + m_v(e)$, then we obtain the vertex– and the edge-PI indices, respectively.[1]

The **edge-PI index** is defined as [16]

$$PI_e = PI_e(G) = \sum_{e=uv} \Big[m_u(e) + m_v(e)\Big] \,.$$

Since this edge version was introduced first, the subscript e is usually omitted and the index is referred to simply as PI index. More details on the PI index are found in the review [17] and the references cited therein.

The **vertex-PI index** seems to was first considered by Khalifeh et al. [18] and is defined as

$$PI_v = PI_v(G) = \sum_{e=uv} \Big[n_u(e) + n_v(e)\Big] \,.$$

The **eccentric connectivity index** of the graph G is defined as [22]

$$Ecc = Ecc(G) = \sum_{u \in V} \deg(u)\, \varepsilon(u) \tag{1.2}$$

where for a given vertex u, its eccentricity $\varepsilon(u)$ is the greatest distance between u and any other vertex of G. The maximum eccentricity over all vertices of G is called the *diameter* of G whereas the minimum eccentricity among the vertices of G is the *radius* of G. The set of vertices whose eccentricity is equal to the radius of G is called the *center* of G. It is well known that each tree has either one or two vertices in its center.

The aim of this article is to contribute to the theory of the above described five topological indices by showing how these can be computed in the case of splice graphs.

Suppose that $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are two graphs with disjoint vertex sets. Let $u_1 \in V_1$ and $u_2 \in V_2$ be given vertices of G_1 and G_2, respectively. Following

[1] The acronym PI comes from Padmakar and Ivan. Whereas Padmakar is the first name of P. V. Khadikar, the inventor of the PI index [16], Ivan comes from the first name of one of the present authors, whose contribution to the discovery of the PI index was nil.

Došlić [4], a splice of G_1 and G_2 at vertices u_1 and u_2, denoted by $\mathcal{S}(G_1, G_2; u_1, u_2)$, is obtained by identifying the vertices u_1 and u_2 in the union of G_1 and G_2 (see Fig. 1).

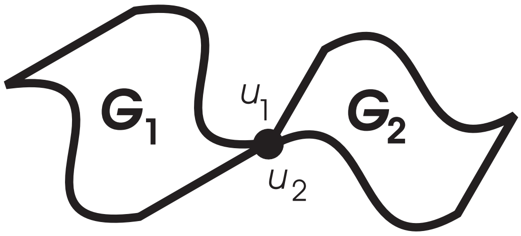

Fig. 1. The splice graph $\mathcal{S}(G_1, G_2; u_1, u_2)$ and the labeling of its structural details.

A variety of topological indices of splice graphs have been computed already in [1,3,19,21]. In this paper we aim at continuing work along the same lines, for a few additional indices. Note that the proof techniques in this article are based on those used in the recent work [20], in which bridge graphs have been examined.

2 Main Results

In this section, we compute the Szeged, edge-Szeged, edge-PI, vertex-PI, and eccentric connectivity indices of the above described splice graph. We first introduce the following structural parameters of $\mathcal{S} = \mathcal{S}(G_1, G_2; u_1, u_2)$. Let $i = 1, 2$ and $f = xy \in E_i$, and

$$\begin{aligned} n_x^i(f) &= \Big|N(f,x,G_i)\Big| \quad , \quad n_y^i(f) = \Big|N(f,y,G_i)\Big| \\ n_x(f) &= \Big|N(f,x,\mathcal{S})\Big| \quad , \quad n_y(f) = \Big|N(f,y,\mathcal{S})\Big| \\ m_x^i(f) &= \Big|M(f,x,G_i)\Big| \quad , \quad m_y^i(f) = \Big|M(f,y,G_i)\Big| \\ m_x(f) &= \Big|M(f,x,\mathcal{S})\Big| \quad , \quad m_y(f) = \Big|M(f,y,\mathcal{S})\Big| \,. \end{aligned}$$

In addition, for a given vertex $u \in V(\mathcal{S})$, let $\varepsilon_1(u)$ be the eccentricity of u as a vertex of G_1, $\varepsilon_2(u)$ the eccentricity of u as a vertex of G_2, and $\varepsilon(u)$ the eccentricity of u as a vertex of the splice graph $\mathcal{S}$.

Proposition 2.1. *Assume that $f = xy \in E_1$.*

(i) If $u_1 \in N(f, x, G_1)$, then

$$n_x(f) = n_x^1(f) + |V_2| \quad , \quad n_y(f) = n_y^1(f)$$
$$m_x(f) = m_x^1(f) + |E_2| \quad , \quad m_y(f) = m_y^1(f) \ .$$

(ii) If $d_{G_1}(u_1, x) = d_{G_1}(u_1, y)$, then

$$n_x(f) = n_x^1(f) \quad , \quad n_y(f) = n_y^1(f)$$
$$m_x(f) = m_x^1(f) \quad , \quad m_y(f) = m_y^1(f) \ .$$

Analogous relations hold if $f = xy \in E_2$.

Proof is easy and is left to the reader.

In order to verify the following propositions we need some preparations. For $i = 1, 2$, let

$$S_i = \Big\{ f = xy \in E_i \,|\, d_{G_i}(x, u_i) = d_{G_i}(y, u_i) \Big\} \quad , \quad T_i = E_i \setminus S_i \quad , \quad t_i = |T_i| \ .$$

In addition, for $f = xy \in E_i$ define

$$n^i(f) = \begin{cases} n_x^i(f) & \text{if} \quad d_{G_i}(x, u_i) > d_{G_i}(y, u_i) \\ n_y^i(f) & \text{if} \quad d_{G_i}(x, u_i) < d_{G_i}(y, u_i) \\ 0 & \text{if} \quad d_{G_i}(x, u_i) = d_{G_i}(y, u_i) \end{cases}$$

and

$$m^i(f) = \begin{cases} m_x^i(f) & \text{if} \quad d_{G_i}(x, u_i) > d_{G_i}(y, u_i) \\ m_y^i(f) & \text{if} \quad d_{G_i}(x, u_i) < d_{G_i}(y, u_i) \\ 0 & \text{if} \quad d_{G_i}(x, u_i) = d_{G_i}(y, u_i) \ . \end{cases}$$

Proposition 2.2.

$$\begin{aligned} Sz(\mathcal{S}) &= Sz(G_1) + Sz(G_2) \\ &+ |V_2| \sum_{f=xy \in E_1} n^1(f) + |V_1| \sum_{f=xy \in E_2} n^2(f) \ . \end{aligned}$$

Proof.

$$
\begin{aligned}
Sz(\mathcal{S}) &= \sum_{f=xy\in E_1} n_x(f)\,n_y(f) + \sum_{f=xy\in E_2} n_x(f)\,n_y(f) \\
&= \sum_{f=xy\in E_1} n^1_x(f)\,n^1_y(f) + \sum_{f=xy\in E_1} |V_2|\,n^1(f) \\
&+ \sum_{f=xy\in E_2} n^2_x(f)\,n^2_y(f) + \sum_{f=xy\in E_2} |V_1|\,n^2(f)\ . \qquad (2.1)
\end{aligned}
$$

Because for $i = 1, 2$,

$$\sum_{f=xy\in E_i} n^i_x(f)\,n^i_y(f) = Sz(G_i)$$

from Eq. (2.1) we directly obtain Proposition 2.2. □

Proposition 2.3.

$$
\begin{aligned}
Sz_e(\mathcal{S}) &= Sz_e(G_1) + Sz_e(G_2) \\
&+ |E_2| \sum_{f=xy\in E_1} m^1(f) + |E_1| \sum_{f=xy\in E_2} m^2(f)\ .
\end{aligned}
$$

Proof.

$$
\begin{aligned}
Sz_e(\mathcal{S}) &= \sum_{f=xy\in E_1} m_x(f)\,m_y(f) + \sum_{f=xy\in E_2} m_x(f)\,m_y(f) \\
&= \sum_{f=xy\in E_1} m^1_x(f)\,m^1_y(f) + \sum_{f=xy\in E_1} |E_2|\,m^1(f) \\
&+ \sum_{f=xy\in E_2} m^2_x(f)\,m^2_y(f) + \sum_{f=xy\in E_2} |E_1|\,m^2(f)\ . \qquad (2.2)
\end{aligned}
$$

Because for $i = 1, 2$,

$$\sum_{f=xy\in E_i} m^i_x(f)\,m^i_y(f) = Sz_e(G_i)$$

from Eq. (2.2) we directly obtain Proposition 2.3. □

Proposition 2.4.

$$PI_v(\mathcal{S}) = PI_v(G_1) + PI_v(G_2) + (t_2+1)|V_1| + (t_1+1)|V_2|\ .$$

Proof.

$$\begin{aligned}
PI_v(\mathcal{S}) &= \sum_{f=xy\in T_1}[n_x(f)+n_y(f)] + \sum_{f=xy\in S_1}[n_x(f)+n_y(f)] \\
&+ \sum_{f=xy\in T_2}[n_x(f)+n_y(f)] + \sum_{f=xy\in S_2}[n_x(f)+n_y(f)] + [n_{u_1}(e)+n_{u_2}(e)] \\
&= \sum_{f=xy\in T_1}[n_x^1(f)+|V_2|+n_y^1(f)] + \sum_{f=xy\in S_1}[n_x^1(f)+n_y^1(f)] \\
&+ \sum_{f=xy\in T_2}[n_x^2(f)+|V_1|+n_y^2(f)] + \sum_{f=xy\in S_2}[n_x^2(f)+n_y^2(f)] + (|V_1|+|V_2|) \\
&= \sum_{f=xy\in T_1}[n_x^1(f)+n_y^1(f)] + t_1\,|V_2| + \sum_{f=xy\in S_1}[n_x^1(f)+n_y^1(f)] \\
&+ \sum_{f=xy\in T_2}[n_x^2(f)+n_y^2(f)] + t_2\,|V_1| + \sum_{f=xy\in S_2}[n_x^2(f)+n_y^2(f)] \\
&+ (|V_1|+|V_2|)\ . \qquad (2.3)
\end{aligned}$$

Because for $i=1,2$,

$$\sum_{f=xy\in T_i}[n_x^i(f)+n_y^i(f)] + \sum_{f=xy\in S_i}[n_x^i(f)+n_y^i(f)] = \sum_{f=xy\in E_i}[n_x^i(f)+n_y^i(f)] = PI_v(G_i)$$

from Eq. (2.3) we directly obtain Proposition 2.4. □

Proposition 2.5.

$$PI(\mathcal{S}) = PI(G_1) + PI(G_2) + t_2\,|E_1| + t_1\,|E_2|\ .$$

Proof.

$$\begin{aligned}
PI(\mathcal{S}) &= \sum_{f=xy\in T_1}[m_x(f)+m_y(f)] + \sum_{f=xy\in S_1}[m_x(f)+m_y(f)] \\
&+ \sum_{f=xy\in T_2}[m_x(f)+m_y(f)] + \sum_{f=xy\in S_2}[m_x(f)+m_y(f)] + [m_{u_1}(e)+m_{u_2}(e)] \\
&= \sum_{f=xy\in T_1}[m_x^1(f)+|E_2|+m_y^1(f)] + \sum_{f=xy\in S_1}[m_x^1(f)+m_y^1(f)] \\
&+ \sum_{f=xy\in T_2}[m_x^2(f)+|E_1|+m_y^2(f)] + \sum_{f=xy\in S_2}[m_x^2(f)+m_y^2(f)]
\end{aligned}$$

$$= \sum_{f=xy\in T_1} [m_x^1(f) + m_y^1(f)] + t_1|E_2| + \sum_{f=xy\in S_1} [m_x^1(f) + m_y^1(f)]$$

$$+ \sum_{f=xy\in T_2} [m_x^2(f) + m_y^2(f)] + t_2|E_1| + \sum_{f=xy\in S_2} [m_x^2(f) + m_y^2(f)] \, .$$

Because for $i = 1, 2$,

$$\sum_{f=xy\in T_i} [m_x^i(f)+m_y^i(f)] + \sum_{f=xy\in S_i} [m_x^i(f)+m_y^i(f)] = \sum_{f=xy\in E_i} [m_x^i(f)+m_y^i(f)] = PI(G_i)$$

from Eq. (2.4) we directly obtain Proposition 2.5. $\square$

Proposition 2.6.

$$\begin{aligned} Ecc(\mathcal{S}) &= \sum_{x\in V_1} \deg_{\mathcal{S}}(x) \cdot \max\left\{d_{G_1}(x,u_1) + \varepsilon_2(u_2),\, \varepsilon_1(x)\right\} \\ &+ \sum_{y\in V_2} \deg_{\mathcal{S}}(y) \cdot \max\left\{d_{G_2}(y,u_2) + \varepsilon_1(u_1)\,,\, \varepsilon_2(y)\right\} \, . \end{aligned}$$

Proof. Consider a vertex x of the splice graph $\mathcal{S}$, such that $x \in V_1$. Let z be the vertex of $\mathcal{S}$ whose distance to x is maximal. Thus, $\varepsilon(x) = d_{\mathcal{S}}(x, z)$. If z belongs to the graph G_1, then $\varepsilon(x) = \varepsilon_1(x)$. If z belongs to the graph G_2, then the distance between x and z is equal to $d_{G_1}(x, u_1) + d_{G_2}(u_2, z)$, see Fig. 1. In addition, z must be the vertex at greatest distance from u_2. Consequently, $\varepsilon(x) = d_{G_1}(x, u_1) + \varepsilon_2(u_2)$. This means that no matter where the vertex z is located,

$$\varepsilon(x) = \max\left\{d_{G_1}(x,u_1) + \varepsilon_2(u_2)\,,\, \varepsilon_1(x)\right\}$$

holds for any vertex $x \in V_1$. The formula for $\varepsilon(y)$ in the case when $y \in V_2$ is fully analogous.

Proposition 2.6 follows now from the definition of the eccentric connectivity index, Eq. (1.2). $\square$

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