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The vertex PI index and Szeged index of bridge graphs

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ABSTRACT

Recently the vertex Padmakar–Ivan (PI_v) index of a graph G was introduced as the sum over all edges $e = uv$ of G of the number of vertices which are not equidistant to the vertices u and v. In this paper the vertex PI index and Szeged index of bridge graphs are determined. Using these formulas, the vertex PI indices and Szeged indices of several graphs are computed.

1. Introduction

In theoretical chemistry molecular structure descriptors – also called topological indices – are used to understand physico-chemical properties of chemical compounds. By now there exist a lot of different types of such indices which capture different aspects of the molecular graphs associated with the molecules considered. Arguably the best known of these indices is the Wiener index [29,12,7,26,27]. The Szeged index [8,15,10] is closely related to the Wiener index and is a vertex-multiplicative type that takes into account how the vertices of a given molecular graph are distributed and coincides with the Wiener index on trees. It has been considered from many points of view, see, e.g., [7,8,10,11,15,17,21–24,26,27,31,33] and the literature given therein. Since the Szeged index takes into account how the vertices are distributed, it is natural to introduce an index that takes into account the distribution of edges. The Padmakar–Ivan (PI) index [14,17] is an additive index that takes into account the distribution of edges and, therefore, complements the Szeged index in a certain sense. It is useful to mention that the PI index is a unique topological index related to parallelism of edges (we will make this more precise below) and it has been studied from many different points of view, see [1–6,9,13,14,16–20,28,30,32]. All the indices mentioned have many chemical applications and it was shown that the PI index correlates well with the Wiener and Szeged indices and that they all correlate with the physico-chemical properties and biological activities of a large number of diverse and complex compounds. Very recently, a new topological index, the vertex PI index, was introduced and some of its properties were derived [25,24,30]. Its definition is similar to that of the (edge) PI index, in that it is additive, but now the distances of vertices (instead of edges) from edges is considered.

In this paper we compute the vertex PI index and the Szeged index for the bridge graph built from a collection of (possibly different) graphs and apply this result to determine the vertex PI index and Szeged index of some classes of graphs.

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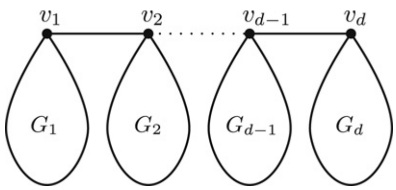

Fig. 1. The bridge graph.

2. Preliminaries

Let G be a connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. As usual, we denote the distance between two arbitrary vertices x and y of G by $d(x, y)$ and it is defined as the number of edges in the minimal path connecting the vertices x and y.

Given an edge $e = uv \in E(G)$ of G, we define the distance of e to a vertex $w \in V(G)$ as the minimum of the distances of its ends to w, i.e.,

$$d(w, e) := \min\{d(w, u), d(w, v)\}.$$

Let us denote the number of vertices lying closer to the vertex u than to the vertex v of e by $n_u(e|G)$ and the number of vertices lying closer to the vertex v than to the vertex u by $n_v(e|G)$. Thus,

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

and similarly for $n_v(e|G)$.

The *vertex Padmakar–Ivan* (PI_v) *index* of a graph G is defined as

$$PI_v(G) := \sum_{e \in E(G)} (n_u(e|G) + n_v(e|G)),$$

see [30,31,33]. Note that in these definitions the vertices equidistant from the two ends of the edge $e = uv$- i.e., vertices a with $d(u, a) = d(v, a)$- are not counted. We also call such vertices *parallel* to e. This implies that we can write

$$PI_v(G) = \sum_{e \in E(G)} n_e(G),$$

where $n_e(G) := n_u(e|G) + n_v(e|G)$ is the number of vertices of G that are not equidistant from the two ends of the edge e.

The *Szeged (Sz) index* of a graph G is defined as

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

Let us briefly recall the definition of bridge graphs. Let $\{G_i\}_{i=1}^d$ be a set of finite pairwise disjoint graphs with $v_i \in V(G_i)$. The *bridge graph* $B(G_1, G_2, \ldots, G_d) = B(G_1, G_2, \ldots, G_d; v_1, v_2, \ldots, v_d)$ of $\{G_i\}_{i=1}^d$ with respect to the vertices $\{v_i\}_{i=1}^d$ is the graph obtained from the graphs $G_1, \ldots, G_d$ by connecting the vertices v_i and v_{i+1} by an edge for all $i = 1, 2, \ldots, d - 1$, see Fig. 1.

The main result of this paper is an explicit formula for the vertex PI index and the Szeged index of a bridge graph of $G_1, \ldots, G_d$.

3. The vertex PI index of the bridge Graph

In order to compute the vertex PI index of the bridge graph $B(G_1, G_2, \ldots, G_d)$ we need the following notation. Let G be any graph and let $v \in V(G)$ be any vertex of G. We denote the set of all edges uu' such that $d(u, v) = d(u', v)$ by $M_v(G)$. The cardinality of $M_v(G)$ is denoted by $m_v(G)$.

Theorem 1. *The vertex PI index of the bridge graph $G = B(G_1, G_2, \ldots, G_d)$ of $\{G_i\}_{i=1}^d$ with respect to the vertices $\{v_i\}_{i=1}^d$ is given by*

$$PI_v(G) = \sum_{i=1}^{d} PI_v(G_i) + (|E(G)| - m(G))|V(G)| - ev(G) + mv(G),$$

where

$$m(G) = \sum_{i=1}^{d} m_{v_i}(G_i), \qquad ev(G) = \sum_{i=1}^{d} |E(G_i)||V(G_i)|, \qquad mv(G) = \sum_{i=1}^{d} m_{v_i}(G_i)|V(G_i)|.$$

Proof. Let $G = B(G_1, G_2, \ldots, G_d)$. From the definitions we have that

$$\begin{aligned} PI_v(G) &= \sum_{e\in E(G)} n_e(G) \\ &= \sum_{i=1}^{d}\sum_{e\in E(G_i)} n_e(G) + \sum_{i=1}^{d-1} n_{v_i v_{i+1}}(G) \\ &= \sum_{i=1}^{d}\sum_{e\in M_{v_i}(G_i)} n_e(G) + \sum_{i=1}^{d}\sum_{e\in E(G_i)\setminus M_{v_i}(G_i)} n_e(G) + \sum_{i=1}^{d-1} n_{v_i v_{i+1}}(G). \end{aligned}$$

If e is the edge $v_i v_{i+1}$ in G, then there exists no vertex a which is equidistant from the ends of the edge e, thus $n_e(G) = |V(G)|$. This implies that

$$PI_v(G) = \sum_{i=1}^{d}\sum_{e\in M_{v_i}(G_i)} n_e(G) + \sum_{i=1}^{d}\sum_{e\in E(G_i)\setminus M_{v_i}(G_i)} n_e(G) + (d-1)|V(G)|.$$

If $e \in M_{v_i}(G_i)$, then all the vertices in $V(G)\setminus V(G_i)$ are equidistant from the ends of the edge e, thus $n_e(G) = n_e(G_i)$, yielding in turn

$$PI_v(G) = \sum_{i=1}^{d}\sum_{e\in M_{v_i}(G_i)} n_e(G_i) + \sum_{i=1}^{d}\sum_{e\in E(G_i)\setminus M_{v_i}(G_i)} n_e(G) + (d-1)|V(G)|.$$

If $e \in E(G_i)\setminus M_{v_i}(G_i)$, then each vertex in $V(G)\setminus V(G_i)$ is not equidistant from the ends of the edge e, thus $n_e(G) = n_e(G_i) + |V(G)| - |V(G_i)|$ and, consequently,

$$PI_v(G) = \sum_{i=1}^{d}\sum_{e\in M_{v_i}(G_i)} n_e(G_i) + \sum_{i=1}^{d}\sum_{e\in E(G_i)\setminus M_{v_i}(G_i)} (n_e(G_i) + |V(G)| - |V(G_i)|) + (d-1)|V(G)|.$$

This is equivalent to

$$\begin{aligned} PI_v(G) &= \sum_{i=1}^{d}\sum_{e\in E(G_i)} n_e(G_i) + \sum_{i=1}^{d}\sum_{e\in E(G_i)\setminus M_{v_i}(G_i)} (|V(G)| - |V(G_i)|) + (d-1)|V(G)| \\ &= \sum_{i=1}^{d} PI_v(G_i) + \sum_{i=1}^{d}(|E(G_i)| - m_{v_i}(G_i))(|V(G)| - |V(G_i)|) + (d-1)|V(G)| \\ &= \sum_{i=1}^{d} PI_v(G_i) + (|E(G)| - m(G) - (d-1))|V(G)| - ev(G) + mv(G) + (d-1)|V(G)| \\ &= \sum_{i=1}^{d} PI_v(G_i) + (|E(G)| - m(G))|V(G)| - ev(G) + mv(G), \end{aligned}$$

as claimed. $\square$

Define

$$G_d(H, v) := B(\underbrace{H, H, \ldots, H}_{d\text{ times}}, \underbrace{v, v, \ldots, v}_{d\text{ times}}).$$

Clearly, $G_1(H, v) = H$ for any vertex v of H. As a corollary of Theorem 1 we have the following result.

Corollary 2. *Let H be any graph with fixed vertex v. Then the vertex PI index of the bridge graph $G_d(H, v)$ is given by*

$$PI_v(G_d(H, v)) = dPI_v(H) + d(d-1)(|E(H)| + 1 - m_v(H))|V(H)|.$$

Proof. Let $G = G_d(H, v)$. Theorem 1 for the bridge graph G gives that

$$PI_v(G) = dPI_v(H) + d(d|E(H)| + d - 1 - dm_v(H))|V(H)| - d(|E(H)| - m_v(H))|V(H)|,$$

which is equivalent to

$$PI_v(G) = dPI_v(H) + d(d-1)(|E(H)| + 1 - m_v(H))|V(H)|,$$

as requested. $\square$

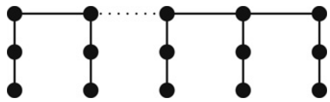

Fig. 2. The graph $A_{d,3}$.

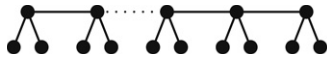

Fig. 3. The graph B_d.

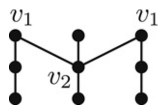

Fig. 4. The graph $B_{3,3;(1,2,1)}$.

Fig. 5. The graph $T_{5,3}$.

For example, let P_m be the path graph on m vertices $v_1, \ldots, v_m$. Clearly, $PI_v(P_m) = m(m-1)$. Let $A_{d,m} := G_d(P_m, v_1)$, see Fig. 2 for $m = 3$. Clearly, $A_{d,1} = P_d$ as well as $A_{1,m} = P_m$.

Corollary 2 for $A_{d,m}$ ($m_{v_1}(P_m) = 0$, $|V(P_m)| = m$, and $|E(P_m)| = m - 1$) gives that

$$PI_v(A_{d,m}) = dm(m-1) + d(d-1)m^2 = dm(dm-1).$$

Note that, in particular, $A_{2,m} = P_{2m}$, implying $PI_v(A_{2,m}) = 2m(2m-1)$ which can be checked directly by inserting $d = 2$ into the above equation.

As another example, define $B_d := G_d(P_3, v_2)$, see Fig. 3 (Polyethene when $d = 4$).

Then Corollary 2 for B_d yields that $PI_v(B_d) = 3d(3d-1)$.

As a first step to generalize this result, we consider the graphs $B_{d,m;l} := G_d(P_m, v_l)$ where we use a path P_m of arbitrary length m and choose a (fixed) vertex v_l (with $1 \leq l \leq m$) in each P_m. Clearly, $B_{d,3;2} = B_d$ from above. Always choosing the first vertex yields the graph $A_{d,m}$, i.e., $B_{d,m;1} = A_{d,m}$ and, hence, $PI_v(B_{d,m;1}) = PI_v(A_{d,m})$. It is easy to check that the vertex PI index of the graph $B_{d,m;l}$ does not depend on the vertex l which we choose in each path (as long as it is the same in each path). Thus, we conclude that

$$PI_v(B_{d,m;l}) = PI_v(B_{d,m;1}) = PI_v(A_{d,m})$$

and the last index has been calculated above. Now, if we want to choose the vertex in each path independently, we cannot use Corollary 2 directly. However, checking the formula given in Theorem 1 we see that – due to $m_v(P_m) = 0$ for any vertex v in P_m – the resulting formula is the same for any choice of vertices in the paths! We describe the result more precisely in the following corollary.

Corollary 3. *Let $\mathcal{I} = (i_1, \ldots, i_d) \in \{1, \ldots, m\}^d$ be a multi-index and denote the bridge graph of d paths P_m joined via the vertices v_{i_k} by $B_{d,m;\mathcal{I}}$, i.e.,*

$$B_{d,m;\mathcal{I}} := B(\underbrace{P_m, \ldots, P_m}_{d\text{ times}}; v_{i_1}, v_{i_2}, \ldots, v_{i_d}).$$

Then the vertex PI index of $B_{d,m;\mathcal{I}}$ is independent of $\mathcal{I}$ and is given by

$$PI_v(B_{d,m;\mathcal{I}}) = dm(dm-1).$$

An example of the graph $B_{3,3;(1,2,1)}$ is shown in Fig. 4.

As a final example, let us consider a graph which is not a tree. Let C_k be the cycle with k vertices and define $T_{d,k} := G_d(C_k, v_1)$, see Fig. 5 when $k = 3$ and $d = 5$.

Corollary 4. *The vertex PI index of $T_{d,k}$ is given by*

$$PI_v(T_{d,k}) = \begin{cases} kd(kd+d-1), & k \text{ is even}, \\ kd(kd-1), & k \text{ is odd}. \end{cases}$$

Proof. Corollary 2 for the bridge graph $T_{d,k}$ states that

$$PI_v(T_{d,k}) = dPI_v(C_k) + d(d-1)\,(k+1-m_v(C_k))\,k,$$

where we have already used the fact that $|E(C_k)| = k = |V(C_k)|$. For k odd one has $PI_v(C_k) = k(k-1)$ and $m_v(C_k) = 1$, whereas for k even one has $PI_v(C_k) = k^2$ and $m_v(C_k) = 0$. Inserting these facts yields the required equations. □

4. The Szeged index of the bridge graph

In this section we derive a formula for the Szeged index of the bridge graph. In order to do that we denote the set of edges $e = uv$ in $E(G_i) \setminus M_{v_i}(G_i)$ such that $d(u, v_i) < d(v, v_i)$ by $L(G_i)$ and the set of edges with $d(u, v_i) > d(v, v_i)$ by $R(G_i)$. To make this well-defined we choose an arbitrary direction on G_i (which we fix for all the following computations) and compute the distances on the underlying graph; the results do not depend on the direction chosen.

Theorem 5. *The Szeged index of the bridge graph $G = B(G_1, G_2, \ldots, G_d)$ of $\{G_i\}_{i=1}^d$, with respect to the vertices $\{v_i\}_{i=1}^d$, is given by*

$$Sz(G) = \sum_{i=1}^{d} Sz(G_i) + \sum_{i=1}^{d-1} \alpha_i(|V(G)| - \alpha_i) + \sum_{i=1}^{d} (|V(G)| - |V(G_i)|)(\ell_i + r_i),$$

where $\alpha_i = \sum_{j=1}^{i} |V(G_j)|$, $\ell_i = \sum_{e=uv\in L(G_i)} n_v(e|G_i)$, and $r_i = \sum_{e=uv\in R(G_i)} n_u(e|G_i)$ for all $i = 1, 2, \ldots, d$.

Proof. Let $G = B(G_1, G_2, \ldots, G_d)$. From the definitions we see that

$$\begin{aligned}
Sz(G) &= \sum_{e=uv\in E(G)} n_u(e|G)n_v(e|G) \\
&= \sum_{i=1}^{d} \sum_{e=uv\in E(G_i)} n_u(e|G)n_v(e|G) + \sum_{i=1}^{d-1} n_{v_i}(v_iv_{i+1}|G)n_{v_{i+1}}(v_iv_{i+1}|G) \\
&= \sum_{i=1}^{d} \sum_{e=uv\in M_{v_i}(G_i)} n_u(e|G)n_v(e|G) \\
&\quad + \sum_{i=1}^{d} \sum_{e=uv\in E(G_i)\setminus M_{v_i}(G_i)} n_u(e|G)n_v(e|G) + \sum_{i=1}^{d-1} n_{v_i}(v_iv_{i+1}|G)n_{v_{i+1}}(v_iv_{i+1}|G).
\end{aligned}$$

If e is the edge v_iv_{i+1} in G, then there exists no vertex a which is equidistant from the ends of the edge $e = v_iv_{i+1}$, thus

$$n_{v_i}(v_iv_{i+1}|G)n_{v_{i+1}}(v_iv_{i+1}|G) = \sum_{j=1}^{i} |V(G_j)| \sum_{j=i+1}^{d} |V(G_j)| = \alpha_i(|V(G)| - \alpha_i).$$

This implies that

$$Sz(G) = \sum_{i=1}^{d} \sum_{e=uv\in M_{v_i}(G_i)} n_u(e|G)n_v(e|G) + \sum_{i=1}^{d} \sum_{e=uv\in E(G_i)\setminus M_{v_i}(G_i)} n_u(e|G)n_v(e|G) + \sum_{i=1}^{d-1} \alpha_i(|V(G)| - \alpha_i).$$

If $e = uv \in M_{v_i}(G_i)$ then all the vertices in $V(G) \setminus V(G_i)$ are equidistant from the ends of the edge $e = uv$, thus $n_u(e|G)n_v(e|G) = n_u(e|G_i)n_v(e|G_i)$, yielding in turn

$$Sz(G) = \sum_{i=1}^{d} \sum_{e=uv\in M_{v_i}(G_i)} n_u(e|G_i)n_v(e|G_i) + \sum_{i=1}^{d} \sum_{e=uv\in E(G_i)\setminus M_{v_i}(G_i)} n_u(e|G)n_v(e|G) + \sum_{i=1}^{d-1} \alpha_i(|V(G)| - \alpha_i).$$

If $e = uv \in E(G_i) \setminus M_{v_i}(G_i)$ then there exist the following two cases:

- $e \in L(G_i)$. In this case we have that

$$n_u(e|G)n_v(e|G) = (n_u(G_i) + |V(G)| - |V(G_i)|)n_v(e|G_i).$$

- $e \in R(G_i)$. In this case we have that

$$n_u(e|G)n_v(e|G) = n_u(G_i)(n_v(e|G_i) + |V(G)| - |V(G_i)|).$$

Therefore,

$$\sum_{i=1}^{d}\sum_{e=uv\in E(G_i)\setminus M_{v_i}(G_i)} n_u(e|G)n_v(e|G) = \sum_{i=1}^{d}\sum_{e=uv\in E(G_i)\setminus M_{v_i}(G_i)} n_u(e|G_i)n_v(e|G_i) + \sum_{i=1}^{d}\sum_{e=uv\in L(G_i)}(|V(G)|-|V(G_i)|)n_v(e|G_i) + \sum_{i=1}^{d}\sum_{e=uv\in R(G_i)}(|V(G)|-|V(G_i)|)n_u(e|G_i).$$

Hence, the Szeged index of the graph G is given by

$$Sz(G) = \sum_{i=1}^{d} Sz(G_i) + \sum_{i=1}^{d-1}\alpha_i(|V(G)|-\alpha_i) + \sum_{i=1}^{d}(|V(G)|-|V(G_i)|)(\ell_i + r_i),$$

as claimed. □

As a corollary of Theorem 5 we have the following result.

Corollary 6. *Let H be any graph with fixed vertex v. Then the Szeged index of the bridge graph $G_d(H, v)$ is given by*

$$Sz(G_d(H,v)) = dSz(H) + \binom{d+1}{3}|V(H)|^2 + d(d-1)|V(H)|(\ell(H)+r(H)),$$

where $\ell(H) = \sum_{e=uv\in L(H)} n_v(e|H)$ and $r(H) = \sum_{e=uv\in R(H)} n_u(e|H)$.

Proof. Let $G = G_d(H, v)$. Theorem 5 for the bridge graph G gives that

$$Sz(G) = dSz(H) + \sum_{i=1}^{d-1} \mathrm{i}(d-\mathrm{i})|V(H)|^2 + \sum_{i=1}^{d}(d-1)|V(H)|(\ell(H)+r(H))$$

which yields after some algebra the assertion. □

Corollary 6 for $A_{d,m}$ ($|V(P_m)| = m$ and $|E(P_m)| = m-1$) gives that

$$Sz(A_{d,m}) = dSz(P_m) + \binom{d+1}{3}m^2 + d(d-1)m(\ell(P_m)+r(P_m)),$$

where $Sz(P_m) = \binom{m+1}{3}$, $\ell(P_m) = 0$ and $r(P_m) = \binom{m}{2}$. Therefore,

$$Sz(A_{d,m}) = d\binom{m+1}{3} + \binom{d+1}{3}m^2 + 2\binom{d}{2}m\binom{m}{2}.$$

Since $A_{2,m} = P_{2m}$ one should have

$$Sz(A_{2,m}) = Sz(P_{2m}) = \binom{2m+1}{3} = \frac{m}{3}(4m^2-1).$$

Inserting $d = 2$ into the above equation yields

$$Sz(A_{2,m}) = 2\binom{m+1}{3} + m^2 + 2m\binom{m}{2} = \frac{m}{3}(4m^2-1),$$

as requested. Considering instead an arbitrary d and $m = 2$ yields

$$Sz(A_{d,2}) = \frac{d}{3}(2d^2+6d-5).$$

Since $A_{d,2}$ is a tree the Szeged index coincides with the Wiener index and the latter has already been given in [10] (there the graph is denoted by F_{2m} and called *fasciagraph*). As another example consider B_d from above. Here we obtain

$$Sz(B_d) = d\binom{3+1}{3} + \binom{d+1}{3}3^2 + d(d-1)3(\ell(P_3)+r(P_3)).$$

However, due to the different vertex with respect to which we define $L(P_3)$ and $R(P_3)$, this time we have $r(P_3) = 1 = \ell(P_3)$, implying

$$Sz(B_d) = \frac{d}{2}(3d^2 + 12d - 7).$$

Again, the Wiener index of this graph (which coincides with the Szeged index) can be found already in [10] (where this graph is denoted by F_{3m}). Now, let us compare $Sz(A_{2,m})$ and $Sz(B_d)$. In the case $m = 3k$ and $d = 2k$ the two graphs $A_{2,3k}$ and B_{2k} have the same number of vertices, namely $6k$. Here one has $Sz(A_{2,3k}) = k(36k^2 - 1)$ and $Sz(B_{2k}) = k(12k^2 + 24k - 7)$. It is clear that $Sz(A_{2,3k}) > Sz(B_{2k})$. More precisely, one has for a large k the fact that $Sz(A_{2,3k}) \sim 3 \cdot Sz(B_{2k})$. The intuitive explanation for this is that $A_{2,3k}$ has a greater diameter than B_{2k}, therefore having more vertices which contribute higher values $n_u(e|G)$ to the sum. More precisely, one has $\mathrm{diam}(A_{2,3k}) = 6k - 1$ and $\mathrm{diam}(B_{2k}) = 2k + 1$, showing that for large k one also has $\mathrm{diam}(A_{2,3k}) \sim 3 \cdot \mathrm{diam}(B_{2k})$. It is, therefore, natural to consider the quotient $\frac{Sz(A_{2,3k})}{\mathrm{diam}(A_{2,3k})} = \frac{k(36k^2-1)}{6k-1} = 6k^2 + k$ as well as

$$\frac{Sz(B_{2k})}{\mathrm{diam}(B_{2k})} = \frac{k(12k^2 + 24k - 7)}{2k + 1} = 6k^2 + 9k - 8 + \frac{8}{2k + 1}$$

which for a very large k nearly coincide.

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