Note on PI and Szeged indices

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Abstract

In theoretical chemistry molecular structure descriptors are used for modeling physico-chemical, pharmacologic, toxicologic, biological and other properties of chemical compounds. In this paper we study distance-based graph invariants and present some improved and corrected sharp inequalities for PI, vertex PI, Szeged and edge Szeged topological indices, involving the number of vertices and edges, the diameter, the number of triangles and the Zagreb indices. In addition, we give a complete characterization of the extremal graphs.

Key words: Molecular descriptors; PI index; Szeged index; Zagreb index; Distance in graphs.

AMS Classifications: 05C12, 92E10.

1 Introduction

Let $G = (V, E)$ be a connected simple graph with $n = |V|$ vertices and $m = |E|$ edges. For vertices $u, v \in V$, the distance $d(u, v)$ is defined as the length of the shortest path between $u$ and $v$ in $G$. The diameter $diam(G)$ is the greatest distance between two vertices of $G$. The distance between the vertex $w$ and the edge $e = uv$ is defined as $d'(w, e) = \min(d(w, u), d(w, v))$.

In theoretical chemistry molecular structure descriptors (also called topological indices) are used for modeling physico-chemical, pharmacologic, toxicologic, biological and other properties of chemical compounds [6]. There exist several types of such indices, especially those based on vertex and edge distances. Arguably the best known of these indices is the Wiener index $W$, defined as the sum of distances between all pairs of vertices of the molecular graph [4, 24],

$$W(G) = \sum_{u, v \in V} d(u, v).$$

Besides of use in chemistry, it was independently studied due to its relevance in social science, architecture and graph theory. With considerable success in chemical graph theory, various extensions and generalizations of the Wiener index are recently put forward [19, 24].

Let $e = uv$ be an edge of the graph $G$. The number of vertices of $G$ whose distance to the vertex $u$ is smaller than the distance to the vertex $v$ is denoted by $n_u(e)$. Analogously, $n_v(e)$ is the number of vertices of $G$ whose distance to the vertex $v$ is smaller than the distance to
the vertex $u$. Similarly, $m_u(e)$ denotes the number of edges of $G$ whose distance to the vertex $u$ is smaller than the distance to the vertex $v$. We now define four topological indices: PI, vertex PI, Szeged and edge Szeged indices of $G$ as follows

$$PI(G) = \sum_{e \in E} m_u(e) + m_v(e)$$

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

$$Sz(G) = \sum_{e \in E} n_u(e) \cdot n_v(e)$$

$$Sz_e(G) = \sum_{e \in E} m_u(e) \cdot m_v(e)$$

Notice that for trees $W(G) = Sz(G)$ and for bipartite graphs $PI_v(G) = nm$.

The paper is organized as follows. In Section 2 we present two improved inequalities on $PI_v$, $PI$, $Sz$ and $Sz_e$ indices, and completely describe the extremal graphs. In Section 3 we prove sharp lower bounds on the vertex PI and Szeged index involving Zagreb indices and correct the equality cases for the upper bound involving the number of triangles. In Section 4 we correct the equality case regarding PI and edge Szeged index and present new sharp bound using Pólya–Szegö inequality.

## 2 Improved inequalities for PI and Szeged indices

Let $X_n$ be the set of graphs on $n$ vertices, such that for every edge $e = uv \in E(G)$ it holds $\min(n_u(e), n_v(e)) = 1$. It is obvious that the complete graph $K_n$ belongs to $X_n$, and we will exclude $K_n$ in the sequel. By simple calculation, $PI_v(K_n) = 2|E(K_n)| = n(n - 1) \text{ and } Sz(G) = |E(K_n)| = \frac{n(n-1)}{2}$.

A chordal graph is a simple graph such that each of its cycles of four or more vertices has a chord, which is an edge joining two vertices that are not adjacent in the cycle.

In [5] the authors stated that a graph $G$ from $X_n$ must be a complete graph or a chordal graph of diameter 2. It follows that the set $X_n$ is composed of the graphs with diameter 2 such that there are no induced path $P_4$ or cycle $C_4$ in the graph $G$. This is the full characterization of graphs from $X_n$.

Namely, let $G$ be a graph with no induced $P_4$ or $C_4$. It follows that diameter of $G$ is less than or equal to two. Since $K_n$ is the unique graph with diameter one, we can assume that diameter of $G$ is equal to 2. Consider an arbitrary edge $e = uv$. Since $G$ does not contain induced $P_4$ or $C_4$, there are no two vertices $u'$ and $v'$ such that $u'$ is a neighbor of $u$, $v'$ is a neighbor of $v$, $d(v, u') > 1$ and $d(u, v') > 1$. Since $diam(G) = 2$, for the vertices $w$ that are not adjacent with $u$ or $v$, it holds $d(v, w) = d(u, w) = 2$. Finally, either $n_u(e) = 1$ or $n_u(e) = 1$.

**Theorem 2.1** Let $G$ be a connected graph with $n$ vertices and $m$ edges. Then

$$PI_v(G) \leq Sz(G) + m,$$

with equality if and only if $G \in X_n$. 

2
Proof. For an arbitrary edge $e = uv$, we have the following inequality
\[
n_v(e) + n_u(e) \leq n_v(e) \cdot n_u(e) + 1,
\]
which is equivalent with $(n_v(e) - 1)(n_u(e) - 1) \geq 0$. By adding similar inequalities for all edges $e \in E(G)$, we get $PI_v(G) \leq S_z(G) + m$. The equality holds if and only if $n_v(e) = 1$ or $n_u(e) = 1$ for all edges $e \in E(G)$, i.e. $G \in X_n$. □

Remark 2.2 The authors in [5] proved the inequality $PI_v(G) \leq 2S_z(G)$. The inequality from Theorem 2.1 is stronger, since $S_z(G) \geq m$.

Remark 2.3 Let $G$ be an arbitrary graph from $X_n$. It can be observed that $G$ contains a vertex with degree $n - 1$. Namely, consider a vertex $v$ with the maximum degree $k < n - 1$. Let $v_1, v_2, \ldots, v_k$ be the neighbors of $v$, and assume that $u$ is not adjacent to $v$. Since the diameter of $G$ is equal to 2, some of the neighbors of $v$ are adjacent to $u$ and let one such vertex be $v_1$. In this case, for $e = vv_1$ it follows $1 = d(v_1, u) < d(v, u) = 2$, and $n_{v_1}(e) \geq 2$. Therefore, $v_1$ must be adjacent to all vertices $v_1, v_2, \ldots, v_p$, which implies that $deg(v_1) > deg(v) = k$. This is impossible, and it follows that $v$ is adjacent to all vertices from $G$.

Let $Y_n$ be the set of graphs on $n$ vertices, such that for every edge $e = uv \in E(G)$ it holds $\min(m_v(e), m_u(e)) = 1$. It is obvious that no graph from $Y_n$ contains pendent vertex (for a pendent vertex $v$ with the only neighbor $u$ it holds $m_v(uv) = 0$). Therefore, the minimum vertex degree of graphs from $Y_n$ is greater than or equal to 2. If all vertices have degree 2, then $G \cong C_n$ and it can be easily seen that only $C_3$ and $C_4$ belong to $Y_n$.

The vertex $v$ is called branching if $deg(v) > 2$. Let $G$ be an arbitrary graph from $Y_n$ and let $v$ be an arbitrary branching vertex. For the edge $vu$ we have $m_v(e) \geq 2$, and it follows that $m_u(e) = 1$. Therefore, all neighbors of the branching vertices have degree two. If $G$ contains exactly one branching vertex $v$, then $G$ is composed of the union of cycles $C_3$ and $C_4$ having the vertex $v$ in common.

Now assume that $G$ contains at least two branching vertices. Let $P_d = w_0w_1 \ldots w_d$ be the shortest path connecting vertices $v$ and $u$, such that $w_0 = v$, $w_d = u$, $deg(v) \geq 3$ and $deg(u) \geq 3$. If $d > 2$, for the edge $e = vv_1$ we have $m_v(e) \geq 2$ and $m_{w_1} \geq 2$ (since the edge $w_2w_3$ is closer to $u$ than to $v$). Therefore, the distance between any two branching vertices is equal to two. If $G$ contains at least three branching vertices, the contradiction follows by considering the edge $e = vu'$ on Fig. 1 (red edges are closer to $u'$ than to $v$). Finally, in this case $G$ contains exactly two branching vertices connected by paths of length two.

The set $Y_{12}$ is presented on Fig. 2.

It can be easily proved by mathematical induction that the number of graphs in $Y_n$ is equal to
\[
|Y_n| = \begin{cases} 
0 & n = 1, 2 \\
1 & n = 3, 4 \\
\left\lfloor \frac{n-1}{6} \right\rfloor + 1, & n \equiv 2 \pmod{6}, \\
\left\lfloor \frac{n-2}{6} \right\rfloor + 2, & \text{otherwise.}
\end{cases}
\]

Remark 2.4 The authors in [5] wrongly stated in Theorem 2 that if $\min(m_u(e), m_v(e)) = 1$ then $G$ is a cycle of length $\leq 4$.

Let $\delta(G)$ denote the minimal vertex degree in the graph $G$.

3
Theorem 2.5 Let $G$ be a connected graph with $n$ vertices, $m$ edges and $\delta(G) \geq 2$. Then
\[ PI(G) \leq Sz_e(G) + m, \]
with equality if and only if $G \in Y_n$.

Proof. The proof is similar to those of Theorem 2.1. The equality holds if and only if $m_{vw}(e) = 1$ or $m_{uw}(e) = 1$ holds for all edges $e \in E(G)$, or equivalently $G \in Y_n$. \hfill \blacksquare

3 Sharp bounds involving Zagreb indices and number of triangles

One of the oldest graph invariants are the first and the second Zagreb indices [6,10], defined as follows
\[ M_1(G) = \sum_{v \in V(G)} \deg(v)^2 \]
\[ M_2(G) = \sum_{uv \in E(G)} \deg(u)\deg(v). \]

Let $t(G)$ denote the number of triangles $K_3$ in the graph $G$.

Proposition 3.1 Let $G$ be a connected graph with diameter 2. Then,
\[ PI_v(G) = M_1(G) - 6t(G). \]
Proof. Let \( e = uv \) be an arbitrary edge, such that it belongs to exactly \( t(e) \) triangles. Adjacent vertices of \( v \) that are not neighbors of \( u \) are closer to \( v \) than \( u \), and vice versa. For the vertices \( w \) that are not neighbors of \( u \) or \( v \), it holds \( d(v, w) = d(u, w) = 2 \). Therefore,

\[
PI_v(G) = \sum_{e \in E(G)} n_u(e) + n_v(e) = \sum_{e \in E(G)} \deg(v) + \deg(u) - 2t(e) = \sum_{v \in V(G)} \deg^2(v) - 2 \sum_{e \in E(G)} t(e) = M_1(G) - 6t(G),
\]

since we counted each triangle three times. This completes the proof.

Remark 3.2 In [21], the authors stated that

\[
n_u(e) + n_v(e) \geq \deg(u) + \deg(v) - t,
\]

where \( t \) is a number such that every edge of \( G \) lie in exactly \( t \) triangles of \( G \). Similarly as in Proposition 3.1, this should be corrected to

\[
n_u(e) + n_v(e) \geq \deg(u) + \deg(v) - 2t(e).
\]

After summing over all edges of \( G \), we get

\[
P_v(G) \geq M_1(G) - 6t(G).
\]

Similarly, we have the following

Proposition 3.3 Let \( G \) be a connected graph with diameter 2, such that every edge belongs to exactly \( t \) triangles. Then,

\[
Sz(G) = M_2(G) - t \cdot M_1(G) + m \cdot t^2.
\]

A graph \( G = SRG(v, k, \lambda, \mu) \) is strongly regular if \( G \) is \( k \)-regular \( v \)-vertex graph such that every two adjacent vertices have \( \lambda \) common neighbors, while every two non-adjacent vertices have \( \mu \) common neighbors. A simple corollary of Proposition 3.1 and Proposition 3.3 is [5]

\[
PI_v(SRG(v, k, \lambda, \mu)) = vk^2 - kv\lambda
\]

\[
Sz(SRG(v, k, \lambda, \mu)) = mk^2 - 2mk\lambda + m\lambda^2.
\]

The following upper bound on the vertex PI index was proved in [2].

Theorem 3.4 Let \( G \) be a connected graph with \( n \) vertices and \( m \) edges. Then,

\[
PI_v(G) \leq nm - 3t(G).
\]
The authors moreover claimed, that the equality holds if an only if $G$ is a bipartite graph or $G \cong K_3$. But this is not true. Namely, the equality holds if and only if for every edge $e = uv$ from $G$ holds $n_u(e) + n_v(e) = n - t(e)$. If $t(G) = 0$, then $PI_v(G) \leq nm$ if and only if $G$ is a bipartite graph. Otherwise, the extremal graph must contain a triangle. For the complete graph it holds

$$n(n - 1) = PI_v(K_n) = n \cdot \binom{n}{2} - 3 \binom{n}{3}.$$  

We checked all graphs on $3 \leq n \leq 10$ vertices with the help of Nauty [20], and the computational results are presented in Table 1, while the extremal graphs with $n = 4, 5, 6$ vertices are presented on Fig. 3. It is interesting that the diameter of all extremal graphs (except $K_n$) is two.

| $n$ | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|-----|---|---|---|---|---|---|---|----|
| count | 1 | 2 | 4 | 7 | 11 | 17 | 25 | 36 |

Table 1: The number of extremal non-bipartite small graphs.

![Figure 3: Non-bipartite extremal graphs for $n = 4, 5, 6$ with $PI_v$ values.](image)

In addition, every extremal graph does not contain induced graph $C_3'$, composed of a triangle with a pendent edge attached to one vertex of a triangle (otherwise the equality $n_u(e) + n_v(e) = n - t(e)$ does not hold).

A graph is odd-hole-free if it has no induced subgraph that is a cycle of odd length greater than 3. Note that the equality holds in Theorem 3.4 for odd-hole-free graphs.

A graph $G$ is a complete $k$-partite graph if there is a partition $V_1 \cup V_2 \cup \ldots \cup V_k = V(G)$ of the vertex set, such that $uv \in E(G)$ if $u$ and $v$ are in different parts of the partition. If $|V_i| = n_i$, then $G$ is denoted by $K_{n_1, n_2, \ldots, n_k}$. It can be easily proved that the equality also holds in Theorem 3.4 for complete $k$-partite graphs $K_{n_1, n_2, \ldots, n_k}$. Namely, consider an arbitrary edge $e = v_i v_j$ that connects parts $V_i$ and $V_j$. The number of triangles that contain the edge $e$ is $n - n_i - n_j$, while $n_u(e) = n_j$ and $n_v(e) = n_i$, and the relation $n_u(e) + n_v(e) = n - t(e)$ holds.

For the completeness, we state the similar result for the Szeged index [3].
Theorem 3.5  Let $G$ be a connected graph with $n$ vertices, $m$ edges and $t(G)$ triangles. Then,

$$Sz(G) \leq \frac{1}{4}n^2m - 3t(G).$$

(1)

If equality holds in (1), then $G$ is bipartite (so in particular $t(G) = 0$), regular, $n$ is even and the minimum vertex degree is greater than 1.

A graph $G$ is distance-balanced if $|n_v(e)| = |n_u(e)|$ holds for any edge $e = uv$ of $G$ (see [12, 18]). In [11] it was proven that a connected bipartite graph $G$ is distance-balanced if and only if $Sz(G) = \frac{1}{4}n^2m$. Recently in [1] the authors presented a simple proof of the conjecture from [17] that the complete balanced bipartite graph $K_{n/2, n/2}$ has maximum Szeged index among all connected graphs with $n$ vertices.

Theorem 3.6  Let $G$ be a connected triangle-free graph with $n \geq 3$ vertices. Then,

$$Sz(G) \geq M_2(G),$$

with equality if and only if $G$ has diameter 2.

Proof.  Let $e = uv$ be an arbitrary edge of $G$. Since $G$ is a triangle-free graph, it follows

$$n_v(e) \cdot n_u(e) \geq \deg(v) \cdot \deg(u).$$

Therefore,

$$Sz(G) = \sum_{e \in E(G)} n_v(e) \cdot n_u(e) \geq \sum_{e \in E(G)} \deg(v) \cdot \deg(u) = M_2(G).$$

Let $G$ be a triangle-tree graph such that $Sz(G) = M_2(G)$. Since $G \nsubseteq K_n$, the diameter of $G$ is greater than or equal to 2. On the other side, if diameter is greater than 2, we can consider induced path $P_4 = w_0w_1w_2w_3$ and for the edge $e = w_0w_1$ it follows that $n_{w_1}(e) > \deg(w_1)$ since $d(w_1, w_3) = 2 < 3 = d(w_0, w_3)$. Therefore, $diam(G) = 2$. In this case, for all vertices $w$ that are on distance greater than one from the vertices $v$ and $u$ holds $d(v, w) = d(u, w) = 2$ and finally $n_v(e) \cdot n_u(e) = \deg(v) \cdot \deg(u)$. This completes the proof. 

4  Further relations

Theorem 4.1  Let $G$ be a connected graph with $n$ vertices and $m$ edges. Then,

$$PI(G) \geq \frac{4}{m-1}SZ_e(G),$$

with equality if and only if $m$ is odd and $G \cong C_n$.

Proof.  Let $e = uv$ be an arbitrary edge of $G$. Using the arithmetic-geometric mean inequality, we have $(m_u(e) + m_v(e))^2 \geq 4m_u(e)m_v(e)$. Therefore,

$$(m - 1)PI(G) = \sum_{e \in E(G)} (m - 1)(m_u(e) + m_v(e)) \geq \sum_{e \in E(G)} (m_u(e) + m_v(e))^2 \geq \sum_{e \in E(G)} 4m_u(e)m_v(e) = 4SZ_e(G).$$
The equality holds if and only if \( m_u(e) = m_v(e) = \frac{m-1}{2} \) for every \( e \in E(G) \). It follows that \( G \) does not have pendant vertices, and therefore \( G \) is not a tree. Finally, \( G \) must contain a cycle, and let \( C = v_1v_2 \ldots v_k \) be the shortest cycle contained in \( G \). If \( k \) is even, by considering the opposite edges we simply get \( m_{v_1}(e) + m_{v_{k+1}}(e) < m-1 \). If \( k \) is odd and \( G \not\cong C_n \), there exist a vertex \( u \) not belonging to \( C \), and without loss of generality suppose that \( u \) is a neighbor of \( v_1 \). In this case \( d(v_{k+1}/2, u_1v) = d(v_{k+3}/2, u_1v) = \frac{k-1}{2} \), and for the edge \( e = v_{k+1}/2v_{k+3}/2 \) we get \( m_{v_{k+1}/2}(e) + m_{v_{k+3}/2}(e) < m-1 \). Therefore, \( k = n \) is odd number and \( G \cong C_n \). ■

**Remark 4.2** In [22], the authors stated in Theorem 4 (b) that 
\[ PI(G) \geq \frac{1}{m-1} \text{SZ}_e(G) \] with equality if and only if \( m = 1 \) is even and \( G \) is a tree with an odd number of vertices or a cycle of odd length.

We will establish another relation between Szeged and vertex PI index, using the following Pólya–Szegö inequality [23].

**Theorem 4.3** Let \( a_1, a_2, \ldots, a_n \) and \( b_1, b_2, \ldots, b_n \) be positive real numbers such that for \( 1 \leq i \leq n \) holds \( a \leq a_i \leq A \) and \( b \leq b_i \leq B \), with \( a < A \) and \( b < B \). Then,
\[
\frac{1}{m} \left( \sum_{i=1}^{n} a_i^2 \right) \cdot \left( \sum_{i=1}^{n} b_i^2 \right) \leq \frac{1}{4} \left( \sqrt{\frac{AB}{ab}} + \sqrt{\frac{ab}{AB}} \right)^2 \cdot \left( \sum_{i=1}^{n} a_i b_i \right)^2.
\]
The equality holds if and only if the numbers
\[
p = \frac{A}{a} + \frac{B}{b} \cdot n \\
q = \frac{B}{a} + \frac{a}{b} \cdot n
\]
are integers, \( a_1 = a_2 = \ldots = a_p = a \), \( a_{p+1} = a_{p+2} = \ldots = a_n = A \), \( b_1 = b_2 = \ldots = b_p = B \) and \( b_{q+1} = b_{q+2} = \ldots = b_n = b \).

**Remark 4.4** By extending the proof of Theorem 4.3, if we allow \( a = A \) or \( b = B \), the equality holds also if \( AB = ab \), i.e. \( a_1 = a_2 = \ldots = a_n = a = A \) and \( b_1 = b_2 = \ldots = b_n = b = B \).

**Theorem 4.5** Let \( G \) be a simple graph with \( n \) vertices and \( m \) edges. Then
\[
32mn \cdot Sz(G) \leq (n+2)^2 \cdot PI^2_G,
\]
with equality if and only if \( m = 0 \) or \( n = 2 \).

**Proof.** Using the arithmetic-geometric mean inequality, it follows
\[
\frac{4}{m} \sum_{e \in E(G)} n_u(e)n_v(e) \leq \sum_{e \in E(G)} \left( n_u(e) + n_v(e) \right)^2. \tag{2}
\]
By setting in Theorem 4.3 the values \( a_i = 1 \) and \( b_i = n_u(e_i) + n_v(e_i) \) for \( i = 1, 2, \ldots, m \), we have
\[
\sum_{i=1}^{m} 1^2 \cdot \sum_{e \in E(G)} \left( n_u(e) + n_v(e) \right)^2 \leq \frac{(AB + ab)^2}{4ABab} \cdot \left( \sum_{e \in E(G)} n_u(e) + n_v(e) \right)^2.
\]
Since $A = a = 1$, we need to estimate upper and lower bounds for $b$, $b = \min_{e \in E(G)} n_u(e) + n_v(e) \geq 2$ and $B = \max_{e \in E(G)} n_u(e) + n_v(e) \leq n$. By analyzing the function $x + \frac{1}{x}$ it follows

$$\frac{(B + b)^2}{4Bb} = \frac{1}{4} \left( \frac{B}{b} + \frac{b}{B} \right) + \frac{1}{2} \leq \frac{(n + 2)^2}{8n}.$$  

Finally, we get

$$m \cdot \sum_{e \in E(G)} (n_u(e) + n_v(e))^2 \leq \frac{(n + 2)^2}{8n} \cdot \left( \sum_{e \in E(G)} n_u(e) + n_v(e) \right)^2. \tag{3}$$

Combining Equations (2) and (3), we complete the proof. The equality holds if and only if $p = \frac{n}{1 + \frac{m}{2}} = \frac{2n}{n + 2}$ is integer or $b = B$, which is possible only for $n = 2$. Therefore, the equality holds if and only if $m = 0$ (in this case $Sz(G) = PI_v(G) = 0$) or $n = 2$.

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