MATCH Communications in Mathematical and in Computer Chemistry

# Some Inequalities for Szeged-Like Topological Indices of Graphs

G. H. Fath-Tabar, M. J. Nadjafi-Arani, M. Mogharrab

Department of Mathematics, Faculty of Science, University of Kashan,

Kashan 87317-51167, Iran

#### A. R. Ashrafi<sup>†</sup>

Department of Mathematics, Faculty of Science, University of Kashan,

Kashan 87317-51167, Iran

School of Mathematics, Institute for Research in Fundamental Sciences (IPM),

P.O. Box: 19395-5746, Tehran, Iran

(Received January 27, 2009)

#### Abstract

The PI, vertex PI and edge Szeged index are three of most important Szegedlike topological indices introduced very recently. The aim of this paper is to present some sharp inequalities between PI, Vertex PI, Szeged and edge Szeged indices of graphs.

### 1 Introduction

Throughout this paper we only consider finite connected graph. Let G be a graph with vertex and edge sets V(G) and E(G), respectively. As usual, the distance between the vertices u and v of G is denoted by  $d_G(u, v)$  (d(u, v) for short) and it is defined as the number of edges in a shortest path connecting the vertices u and v.

<sup>\*</sup>Corresponding author (E-mail: fathtabar@kashanu.ac.ir).

<sup>&</sup>lt;sup>†</sup>This author was in part supported by a grant from IPM (No. 87200113).

Suppose *Graph* denotes the class of all graphs. A map *Top* from *Graphs* into real numbers is called a topological index, if  $G \cong H$  implies that Top(G) = Top(H). The Wiener index was the first reported topological index based on graph distances, see [28]. This index is defined as the sum of all distances between vertices of the graph under consideration, see for detail [7, 8].

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. The edge variants of  $n_u(e)$  and  $n_v(e)$ are denoted by  $m_u(v)$  and  $m_v(e)$ , respectively. We now define four topological indices of the PI, vertex PI, Szeged and edge Szeged indices of the graph G as follows:

$$PI(G) = \sum_{e=uv} [m_u(e) + m_v(e)] \quad ([20, 19, 3]),$$
  

$$PI_v(G) = \sum_{e=uv} [n_u(e) + n_v(e)] \quad ([22, 23, 1, 29])$$
  

$$Sz(G) = \sum_{e=uv} [n_u(e) \cdot n_v(e)] \quad ([12]),$$
  

$$Sz_e(G) = \sum_{e=uv} [m_u(e) \cdot m_v(e)] \quad ([13, 21, 27]).$$

These topological indices attracted recently much attention [2, 4, 5, 9, 10, 11, 14, 15, 16, 17, 18, 24, 25].

Define  $N_G(u)$  to be the set of all vertices adjacent to u. The diameter diam(G) is the greatest distance between two vertices of G. The complete graph on vertices is denoted by  $K_n$ . Other notations are standard and taken mainly from [6, 26].

## 2 Main Results

A graph G is called k-regular if  $deg_G(v) = k$ , for all  $v \in V(G)$ ; a regular graph is one that is k-regular for some k. A k-regular graph G is said to be strongly regular with parameters (v, k, r, s) if |v(G)| = v, any two adjacent vertices of G have exactly r common neighbors and any two non-adjacent vertices of G have exactly s common neighbors. In this case, we denote G by Srg(v, k, r, s). It is well-known that if G is strongly regular with parameters (v, k, r, s) then r > 0. Moreover, strongly regular graphs have diameter 2.

**Theorem 1.** Let G = Srg(v, k, r, s) be a connected graph. Then  $PI_v(G) = kv(k-r)$ 

and  $Sz(G) = m(k - r)^2$ .

**Proof.** Let G be a strongly regular graph with parameters (v, k, r, s). It is easy to see that s = 0 if and only if G is a graph in which its components are complete graphs with the same vertices. Since G is connected,  $G \cong K_v$ , as desired. Suppose  $s \ge 1$  and e = uv is an edge of G. Define  $A_e$  to be the set of all vertices which are equidistant from u and v. Choose a vertex x outside  $N_G(u) \cup N_G(v)$ . Since strongly regular graphs have diameter 2, d(u, x) = d(v, x) = 2. Thus  $n_u(e) = n_v(e) = k - r$ . Therefore,  $PI_v(G) = kv(k - r)$  and  $Sz(G) = m(k - r)^2$ .

A chordless cycle C of a graph H is a graph cycle of length at least four such that the graph cycle is an induced subgraph. A chordal graph is a simple graph possessing no chordless cycles.

#### **Theorem 2.** Suppose G is a graph.

(a) If for every  $e = uv \in E(G)$ ,  $Min\{n_u(e), n_v(e)\} = 1$  then G is complete or a chordal graph of diameter 2.

(b) If  $Min\{m_u(e), m_v(e)\} = 1$  then G is a cycle of length  $\leq 4$ .

**Proof.** (a) Suppose G is not chordal. Then there is a chordless cycle  $C : u_1, u_2, \ldots, u_n, u_1$ . Consider the edge  $e = u_2u_3 \in C$ . Since  $d(u_1, u_2) < d(u_1, u_3 \text{ and } d(u_3, u_4) < d(u_3, u_1)$ ,  $Min\{n_u(e), n_v(e)\} > 1$  lead to a contradiction. So G is chordal. If  $diam(G) \ge 3$  then there are vertices u and v such that d(u, v) = 3. Consider the path P : u, w, z, v in G. Since d(u, w) < d(u, v) and d(z, v) < d(z, u),  $Min\{n_u(wz), n_v(wz)\} > 1$  lead again to a contradiction. So diam(G) = 2 and the proof is complete. The proof of part (b) is the same as (a).  $\Box$ 

**Theorem 3.** Let G be connected graph with exactly n and m vertices and edges, respectively. Then the following statements are holds:

(a)  $PI_v(G) \leq 2Sz(G)$  with equality if and only if G is a complete graph.

(b)  $PI_v(G) \ge \frac{4}{n}Sz(G)$  with equality if and only if n is even and G is the complete bipartite graph  $K_{\frac{n}{2},\frac{n}{2}}$ .

(c)  $PI_v(G)^2 > 4Sz(G)$ ,  $PI_v(G)^2 > (2m + 2Sz(G) \text{ and } P_v(G)^2 > PI_v(G) + 2Sz(G)$ .

(d) If for each edge  $e = uv \in E(G)$ ,  $Min\{n_u(e), n_v(e)\} = 1$  then  $PI_v(G) > Sz(G)$ .

(e) If for each edge  $e = uv \in E(G)$ ,  $Min\{n_u(e), n_v(e)\} > 1$  then  $PI_v(G) < Sz(G)$ .

**Proof.** (a) Since for every edge e = uv,  $n_u(e) + n_v(e) \le 2n_u(e)n_v(e)$ ,  $PI_v(G) \le 2n_u(e)n_v(e)$ 

2Sz(G). The equality is satisfied if and only if for each edge e = uv,  $n_u(e) = n_v(e) = 1$  if and only if G is complete. To prove (b), we notice that  $(n_u(e) + n_v(e))^2 \ge 4n_u(e)n_v(e)$ . Thus,

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

$$\geq \sum_{e=uv} [n_u(e) + n_v(e)]^2$$
  

$$\geq \sum_{e=uv} 4n_u(e)n_v(e) = 4Sz(G) .$$

γ

Obviously, the equality is satisfied if and only if  $n_u(e) = n_v(e) = \frac{n}{2}$ , for each edge e = uv, if and only if G is a complete bipartite graph  $K_{\frac{n}{2},\frac{n}{2}}$ . On the other hand,  $PI_v(g)^2 \geq \sum_{e=uv} [n_u(e) + n_v(e)]^2 \geq 4Sz(G)$ , leads to the proof of (c). Other parts of (c) are obtained in a similar way. To prove (d), it is enough to notice that if  $Min\{n_u(e), n_v(e)\} = 1$  then  $n_u(e) + n_v(e) > n_u(e)n_v(e)$ . Hence  $PI_v(G) > Sz(G)$ . The proof of (e) is similar to (d) and it is omitted.

**Theorem 4.** Let G be n-vertex connected graph. Then the following statements are holds:

(a) If  $Min_{e=uv\in E(G)}\{m_u(e), m_v(e)\} \geq 1$  then for each edge  $e = uv \in E(G)$ ,  $Min\{m_u(e), m_v(e)\} \geq 1$  then  $PI(G) \leq 2Sz_e(G)$  with equality if and only if G is a cycle graph of length  $\leq 4$ .

(b)  $PI(G) \ge \frac{4}{m-1}Sz_e(G)$  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.

(c)  $PI(G)^2 > 4Sz_e(G)$  and if  $Min_{e=uv \in E(G)} \{m_u(e), m_v(e)\} \ge 1$  then  $PI(G)^2 > (2m + 2Sz(G))$ .

(d) If for each edge  $e = uv \in E(G)$ ,  $Min\{m_u(e), m_v(e)\} = 1$  then  $PI(G) > Sz_e(G)$ .

(e) If for each edge  $e = uv \in E(G)$ ,  $Min\{m_u(e), m_v(e)\} > 1$  then  $PI(G) < Sz_e(G)$ .

(f) If for each edge  $e = uv \in E(G)$ ,  $Min\{m_u(e), m_v(e)\} = 0$  then G is isomorphic to  $K_2$ .

**Proof.** The proof is similar to those of Theorem 3 and is omitted.

## References

- A. R. Ashrafi, M. Ghorbani, M. Jalali, The vertex PI and Szeged polynomials of an infinite family of fullerenes, J. Theor. Comput. Chem. 7 (2008) 221–231.
- [2] A. R. Ashrafi, M. Jalali, M. Ghorbani, M. V. Diudea, Computing PI and omega polynomials of an infinite family of fullerenes, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 905–916.
- [3] A. R. Ashrafi, A. Loghman, PI index of armchair polyhex nanotubes, Ars Comb. 80 (2006) 193–199.
- [4] A. R. Ashrafi, M. Mirzargar, The edge Szeged polynomial of graphs, MATCH Commun. Math. Comput. Chem. 60 (2008) 897–904.
- [5] H. Deng, On the PI index of a graph, MATCH Commun. Math. Comput. Chem. 60 (2008) 649–657.
- [6] M. V. Diudea, I. Gutman, L. Jantschi, *Molecular Topology*, Huntington, NY, 2001.
- [7] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, Acta Appl. Math. 66 (2001) 211–249.
- [8] A. A. Dobrynin, I. Gutman, S. Klavžar, P. Žigert., Wiener index of hexagonal systems, Acta Appl. Math. 72 (2002) 247–294.
- [9] M. Eliasi, B. Taeri, Szeged index of armchair polyhex nanotubes, MATCH Commun. Math. Comput. Chem. 59 (2008) 437–450.
- [10] M. Eliasi, B. Taeri, Distance in armchair polyhex nanotubes, MATCH Commun. Math. Comput. Chem. 62 (2009) 295–310.
- [11] M. Ghorbani, M. Jalali, The vertex PI, Szeged and omega polynomials of carbon nanocones CNC<sub>4</sub>[n], MATCH Commun. Math. Comput. Chem. **62** (2009) 353– 362.
- [12] I. Gutman, A formula for the Wiener number of trees and its extension to graphs. containing cycles, *Graph Theory Notes New York* 27 (1994) 9-15.
- [13] I. Gutman, A. R. Ashrafi, The Edge version of the Szeged index, Croat. Chem. Acta 81 (2008) 263–266.
- [14] I. Gutman, A. R. Ashrafi, On the PI index of phenylenes and their hexagonal squeezes, MATCH Commun. Math. Comput. Chem. 60 (2008) 135–142.

- [15] J. Hao, Some bounds for PI indices, MATCH Commun. Math. Comput. Chem. 60 (2008) 121–134.
- [16] A. Iranamanesh, N. A. Gholami, Computing the Szeged index of styrylbenzene dendrimer and triarylamine dendrimer of generation 1–3, *MATCH Commun. Math. Comput. Chem.* 62 (2009) 371–379.
- [17] A. Iranmanesh, I. Gutman, O. Khormali, A. Mahmiani, The edge versions of the Wiener index, MATCH Commun. Math. Comput. Chem. 61 (2009) 663–672.
- [18] A. Iranamanesh, A. S. Kafrani, Computation of the first edge-Wiener index of  $TUC_4C_8(S)$  nanotube, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 311–352.
- [19] P. V. Khadikar, S. Karmarkar, V. K. Agrawal, A novel PI index and its applications to QSPR/QSAR studies, J. Chem. Inf. Comput. Sci. 41 (2001) 934–949.
- [20] P. V. Khadikar, On a novel structural descriptor PI, Nat. Acad. Sci. Lett. 23 (2000) 113–118.
- [21] M. H. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, I. Gutman, The edge Szeged index of product graphs, *Croat. Chem. Acta* 81 (2008) 277–281.
- [22] M. H. Khalifeh, H. Yousefi–Azari, A. R. Ashrafi, Vertex and edge PI indices of Cartesian product graphs, *Discr. Appl. Math.* **156** (2008) 1780–1789.
- [23] M. H. Khalifeh, H. Yousefi–Azari, A. R. Ashrafi, A matrix method for computing Szeged and vertex PI indices of join and composition of graphs, *Lin. Algebra Appl.* **429** (2008) 2702–2709.
- [24] T. Mansour, M. Schork, The PI index of bridge and chain graphs, MATCH Commun. Math. Comput. Chem. 61 (2009) 723–734.
- [25] M. Mirzagar, PI, Szeged and edge Szeged polynomials of a dendrimer nanostar, MATCH Commun. Math. Comput. Chem. 62 (2009) 363–370.
- [26] N. Trinajstić, Chemical Graph Theory, CRC Press, Boca Raton, 1992.
- [27] D. Vukičević, Note on the graphs with the greatest edge-Szeged index, MATCH Commun. Math. Comput. Chem. 61 (2009) 673–681.
- [28] H. Wiener, Structural determination of the paraffin boiling points, J. Am. Chem. Soc. 69 (1947) 17–20.
- [29] H. Yousefi-Azari, A. R. Ashrafi, M. H. Khalifeh, Computing vertex-PI index of single and multi-walled nanotubes, *Digest Journal of Nanomaterials and Biostructures* 3 (2008) 315–318.