CROATICA CHEMICA ACTA CCACAA **70** (3) 819–825 (1997)

ISSN–0011-1643
CCA–2456

Original Scientific Paper

Graphs Having the Maximal Value of the Szeged Index

Andrey A. Dobrynin

Sobolev Institute of Mathematics, Siberian Branch of the Russian Academy of Sciences, Novosibirsk 630090, Russia

Received November 4, 1996; revised February 4, 1997; accepted February 13, 1997

The Szeged index is a new topological index based on distances between the vertices of a graph. The conjecture of Klavžar, Rajapakse and Gutman concerning graphs with the maximal value of the Szeged index is proved. More precisely, a complete bipartite graph $K_{[p/2],[(p+1)/2]}$ has the maximum Szeged index among all the connected graphs on p vertices.

INTRODUCTION

Almost fifty years ago, H. Wiener introduced a topological index based on the distances between carbon atoms in alkanes.[1] Nowadays, this index is referred to as the Wiener number (or Wiener index).[2] The best-known generalization of the Wiener index (W) for arbitrary graphs was proposed by Hosoya.[3] According to his considerations, W is the sum of distances between all pairs of vertices of a connected graph. Another generalization of the Wiener index for cyclic graphs has been recently put forward by Gutman:[4]

$$Sz(\mathrm{G}) = \sum_{(u,v)} n_u n_v, \qquad (1)$$

where the summation goes over all edges (u,v) in an arbitrary connected graph G, $n_u = |\{w|d(w,u) < d(w,v)\}|$, $n_v = |\{w|d(w,v) < d(w,u)\}|$ and the distance $d(u,v)$ is the number of edges in the shortest path connecting vertices u,v in G. It has been demonstrated that in the case of trees the quantities Sz and W coincide.[4] In the case of arbitrary graphs, there are vertices equidistant to both ends of an edge. By definition of Sz, such vertices are not taken into account. An example illustrating the calculation of Sz is shown in Figure 1. The Szeged index of G is equal to the sum of the following edge contributions: $n_{v1}n_{v2} = 1 \times 1 = 1$, $n_{v1}n_{v3} = 1 \times 3 = 3$, $n_{v2}n_{v3} = 1 \times 3 = 3$, $n_{v3}n_{v4} = 3 \times 2 = 6$, and $n_{v4}n_{v5} = 4 \times 1 = 4$. This gives $Sz(G) = 17$.

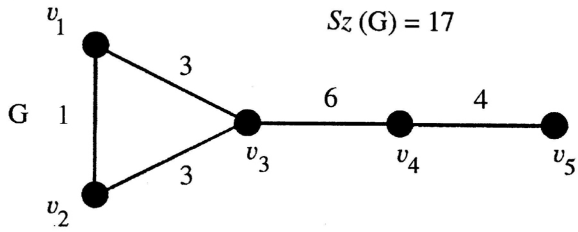

Figure 1. Edge contributions to the Szeged index.

Mathematical properties and chemical applications of *Sz* have been described in recent works.[4–16] It has been established that $Sz(G) \geq W(G)$ for all connected graphs and $Sz(G) = W(G)$ if and only if all blocks of G are complete (note that every block of a tree is a two-vertex complete graph).[4,6] This implies that a complete graph K_p has the minimum Szeged index among all the graphs on *p* vertices. Indeed, suppose that G is not isomorphic to K_p. Then

$$Sz(G) \geq W(G) > W(K_p) = Sz(K_p).$$

Therefore, the minimal value of the Szeged index is equal to $Sz(K_p) = \sum_{(u,v)} 1 \cdot 1 = q(K_p) = p(p-1)/2$.

Denote the complete bipartite graph $K_{[p/2],[(p+1)/2]}$ by K, where $[n]$ is the greatest integer not larger than *n*. It has been shown that $Sz(K) > Sz(G)$ for any bipartite graph G with *p* vertices[4] and the following conjecture has been recently proposed:[10]

CONJECTURE. *The bipartite graph K has the maximum Szeged index among all (connected) graphs on p vertices.*

Within this paper we prove the above conjecture.

STATEMENT OF THE RESULT

By definition of *Sz*, every edge of a graph makes a positive contribution to *Sz*. Graph K has only $[p^2/4]$ edges. In spite of this, the following result shows that K has the maximum Szeged index.

THEOREM. *If graphs G and K have the same number of vertices and G is not isomorphic to K, then* Sz*(G)* < Sz*(K).*

Thus the Szeged index of a graph G lies between $Sz(K_p)$ and $Sz(K)$. This defines an interval of possible values of Sz and allows examination of the isomer degeneracy and the related questions for the Szeged index.

SOME AUXILIARY RESULTS

Let G be an arbitrary graph with p vertices and q edges. For an edge (u,v) of G, we define $n_{uv} = |\{w|d(w,v) = d(w,u)\}|$. It is easy to see that $0 \leq n_{uv} \leq p-2$ and for any edge (u,v) of G, $n_u + n_v = p - n_{uv}$ and $4n_un_v = (n_u+n_v)^2 - (n_u-n_v)^2$. Substituting these expressions into (1), the following useful formula for Sz can be derived.

PROPOSITION 1. *For an arbitrary graph G,*

$$Sz(G) = \frac{1}{4}\left(p^2q - \sum_{(u,v)} n_{uv}(2p-n_{uv}) - \sum_{(u,v)} (n_u-n_v)^2\right). \tag{2}$$

Let (u,v) be an edge of K. Then $n_{uv} = 0$, $n_u = n_v = p/2$ if p is even and $n_u = (p-1)/2$, $n_v = (p+1)/2$ if p is odd. Therefore, the Szeged index for K is immediately obtained.

PROPOSITION 2. *For the complete bipartite graph K,* $Sz(K) = p^2q/4 = p^4/16$ *if p is even;* $Sz(K) = (p^2-1)q/4 = (p^2-1)^2/16$ *if p is odd.*

Denote by t(G) the number of triangles (cycles on three vertices) of a graph G. The proof of the conjecture is based on the estimation of t(G) for graphs with a large number of edges. Further, the following results will be used.

PROPOSITION 3. *For the number of triangles of G,*

$$q(4q-p^2)/p \leq 3t(G) \leq \sum_{(u,v)} n_{uv}. \tag{3}$$

The first inequality is due to Bollobás.[17] Since n_{uv} counts cycles of odd length containing an edge (u,v), the second inequality is obvious.

PROPOSITION 4. *If G has the number of edges* $q(G) \geq [p^2/4] + m$ *and* $1 \leq m \leq [(p-1)/2]$, *then*

$$t(G) \geq m[p/2]. \tag{4}$$

This inequality was given by Nikiforov, Khadzhiivanov[18] and Lovász, Simonovits.[19]

PROOF OF THE THEOREM

Two cases are distinguished:

(a). Let $q(G) \leq q(K)$.

Note that K has the maximal number of edges among all the bipartite graphs with p vertices. Since $1 \leq n_u, n_v \leq p-1$, the maximal value of the product $n_u n_v$ is equal to $[p/2] \cdot [(p+1)/2]$. This extreme value is realized by every edge (u,v) of K. If an edge (x,y) belongs to a cycle of odd length in G, then $n_{xy} > 0$ and, consequently, $n_x n_y < n_u n_v$. It is easy to verify that these properties imply $Sz(G) < Sz(K)$.

(b). Let $q(G) > q(K)$.

Suppose that p is even, *i.e.*, $q(G) = q(K) + m = p^2/4 + m$, where $m > 0$. In this case the equality (2) is applied. Then, one obtains

$$
\begin{aligned}
4[Sz(G) - Sz(K)] &= p^2 q(G) - \sum_{(u,v)} n_{uv}(2p-n_{uv}) - \sum_{(u,v)} (n_u-n_v)^2 - p^2 q(K) \\
&= p^2 m - \sum_{(u,v)} n_{uv}(2p-n_{uv}) - \sum_{(u,v)} (n_u-n_v)^2 \\
&\leq p^2 m - \sum_{(u,v)} n_{uv}(2p-n_{uv}) \\
&\leq p^2 m - \sum_{(u,v)} n_{uv}(2p - (p-2)) \\
&= p^2 m - (p+2) \sum_{(u,v)} n_{uv} \\
&\leq p^2 m - (p+2)\, 3t(G).
\end{aligned}
$$

Then, by Proposition 3

$$
\begin{aligned}
4[Sz(G) - Sz(K)] &\leq p^2 m - (p+2) q(4q-p^2)/p \\
&= p^2 m - (p+2)(p^2/4+m)4m/p \\
&= p^2 m - 4m(p^2/4+m) \\
&= -4m^2 < 0.
\end{aligned}
$$

Suppose now that p is odd, *i.e.*, $q(G) = q(K) + m = (p^2-1)/4+m$ and $m > 0$. If $p = 3$, then G is a triangle and $Sz(K) = Sz(K_{1,2}) = Sz(G)+1$. Further, $p \geq 5$ is assumed. For odd p, two cases can be considered.

Let $m > (p-1)/2$. Then

$$4[Sz(G) - Sz(K)] = p^2q(G) - \sum_{(u,v)} n_{uv}(2p-n_{uv}) - \sum_{(u,v)} (n_u-n_v)^2 - (p^2-1)q(K)$$

$$\leq p^2m + q(K) - \sum_{(u,v)} n_{uv}(2p-n_{uv})$$

$$= p^2m + q(K) - (p+2)\sum_{(u,v)} n_{uv}$$

$$\leq p^2m + q(K) - (p+2)\, 3t(G).$$

Applying Eq. (3) again, one obtains

$$4[Sz(G) - Sz(K)] \leq p^2m + (p^2-1)/4 - (p+2)q(4q-p^2)/p$$

$$< p^2m + (p^2-1)/4 - [(p^2-1)/4+m]\,(4m-1)$$

$$= (p^2-1)/2 - 2m(2m-1)$$

$$< (p^2-1)/2 - (p-1)(p-2)$$

$$= -(p-1)(p-5)/2 \leq 0.$$

Let $1 \leq m \leq (p-1)/2$. Then, as in the previous case

$$4[Sz(G) - Sz(K)] \leq p^2m + q(K) - (p+2)\, 3t(G).$$

Applying Eq. (4) for the number of triangles, one obtains

$$4[Sz(G) - Sz(K)] \leq p^2m + (p^2-1)/4 - (p+2)\, 3m(p-1)/2$$

$$\leq p^2/4 - p^2m/2$$

$$= p^2(1-2m)/4 < 0.$$

CONCLUSION

In this paper, the exact upper bound for the Szeged index has been established. The extreme values of the Szeged index are still unknown for some special classes of graphs, for instance, for bicyclic and planar graphs.[4] Note that the extreme values of Sz for unbranched hexagonal chains have been found.[9] In conclusion we point out the difference between Sz and W. It is a well-known fact that the simple path has the maximum Wiener index among all the graphs having the same number of vertices.

Acknowledgement. – The author is grateful to the referees for their valuable remarks and suggestions.

REFERENCES

1. H. Wiener, *J. Am. Chem. Soc.* **69** (1947) 17.
2. N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1992.
3. H. Hosoya, *Bull. Chem. Soc. Japan* **44** (1971) 2332.
4. I. Gutman, *Graph Theory Notes New York* **27** (1994) 9.
5. A. A. Dobrynin and I. Gutman, *Publ. Inst. Math. (Beograd)* **56** (1994) 18.
6. A. A. Dobrynin and I. Gutman, *Graph Theory Notes New York* **28** (1995) 21.
7. P. V. Khadikar, N. V. Deshpande, P. P. Kale, A. A. Dobrynin, I. Gutman, and G. Dömötör, *J. Chem. Inf. Comput. Sci.* **35** (1995) 574.
8. A. A. Dobrynin, I. Gutman, and G. Dömötör, *Appl. Math. Lett.* **8** (1995) 57.
9. A. A. Dobrynin and I. Gutman, *Croat. Chem. Acta* **69** (1996) 845.
10. S. Klavžar, A. Rajapakse, and I. Gutman, *Appl. Math. Lett.* **9** (1996) 45.
11. A. A. Dobrynin and I. Gutman, *MATCH* **35** (1997), in press.
12. I. Gutman, P. V. Khadikar, P. V. Rajput, and S. Karmarkar, *J. Serb. Chem. Soc.* **60** (1995) 759.
13. P. V. Khadikar, S. Karmarkar, S. Joshi, and I. Gutman, *J. Serb. Chem. Soc.* **61** (1996) 89.
14. J. Žerovnik, *Croat. Chem. Acta* **69** (1996) 837.
15. I. Gutman, *Bull. Acad. Serbe Sci. Arts Cl. Sci. Math. Natur.* **111** (1996) 19.
16. A. A. Dobrynin, *MATCH* **35** (1997), in press.
17. B. Bollobás, *Extremal Graph Theory*, Academic Press, London, 1978, p. 297.
18. V. S. Nikiforov and N. G. Khadzhiivanov, *C. R. Acad. Bulg. Sci.* **34** (1981) 969.
19. L. Lovász and M. Simonovits, *Studies Pure Math.* (1983) 459.

SAŽETAK

Grafovi s maksimalnom vrijednošću Szegedova indeksa

Andrey A. Dobrynin

Szegedov indeks novi je topološki indeks utemeljen na udaljenosti čvorova u grafu. Dokazana je Klavžar-Rajapakse-Gutmanova pretpostavka o grafovima s maksimalnom vrijednoću Szegedova indeksa: od svih povezanih grafova s p čvorova potpun bipartitni graf $K_{[p/2],[(p+1)/2]}$ ima maksimalni Szegedov indeks.