Pergamon

Appl. Math. Lett. Vol. 9, No. 5, pp. 45–49, 1996

0893-9659/96 $15.00 + 0.00

PII: S0893-9659(96)00071-7

The Szeged and the Wiener Index of Graphs

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(Received and accepted January 1996)

Abstract—The Szeged index Sz is a recently introduced graph invariant, having applications in chemistry. In this paper, a formula for the Szeged index of Cartesian product graphs is obtained and some other composite graphs are considered. We also prove that for all connected graphs, Sz is greater than or equal to the sum of distances between all vertices. A conjecture concerning the maximum value of Sz is put forward.

Keywords—Distance in graphs, Wiener number, Szeged index, Graph products.

1. INTRODUCTION

In recent research in mathematical chemistry, particular attention is paid to distance-based graph invariants. The oldest and most thoroughly examined such invariant is the Wiener index (or Wiener number) W; for details on its theory see the review [1]. Another, newly introduced invariant of the same kind is the Szeged index [2] Sz. A few basic mathematical properties of Sz were established [2–5] and its certain chemical applications reported [6,7].

Graphs considered in this paper are finite, **connected** and undirected, without loops or multiple edges. For a graph G, let $V(G)$ and $E(G)$ denote its vertex set and edge set, respectively. The number of vertices of G will be denoted by $|G|$ and $d_G(v)$ will stand for the degree of a vertex v in G.

Let $d_G(u,v)$ be the number of edges in a shortest path between vertices u and v in a graph G. Then the *Wiener index* of a graph G, $W(G)$ is defined as $W(G) = 1/2 \sum_{u,v \in V(G)} d_G(u,v)$.

Let $e = uv$ be an edge of a graph G. Let $N_1(e \mid G)$ be the vertices of G which are closer to u than to v and let $N_2(e \mid G)$ be those vertices which are closer to v than to u. More formally, $N_1(e \mid G) = \{w \mid w \in V(G), d_G(w,u) < d_G(w,v)\}$ and $N_2(e \mid G) = \{w \mid w \in V(G), d_G(w,v) < d_G(w,u)\}$. Let $n_1(e \mid G) = |N_1(e \mid G)|$ and $n_2(e \mid G) = |N_2(e \mid G)|$. Then the *Szeged index* of a

*Supported by the Ministry of Science and Technology of Slovenia under the Grant J1-7036/94.
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graph G, denoted by $Sz(G)$, is defined as

$$Sz(G) = \sum_{e \in E(G)} n_1(e \mid G) n_2(e \mid G).$$

Notice that in the previous works, [2–5] the symbol W^* was used instead of Sz, and no name for the respective graph invariant was put forward.

The *Cartesian product* $G \times H$ of graphs G and H has the vertex set $V(G \times H) = V(G) \times V(H)$ and $(a, x)(b, y)$ is an edge of $G \times H$ if $a = b$ and $xy \in E(H)$, or $ab \in E(G)$ and $x = y$. Note that each edge of $G \times H$ is either contained in an (isomorphic) copy of G or in an (isomorphic) copy of H. Observe also that in $G \times H$, there are $|H|$ isomorphic copies of G and $|G|$ isomorphic copies of H. The Cartesian product is associative and commutative. Furthermore, it is connected if and only if both factor graphs are connected.

The Wiener index of Cartesian product graphs was studied in [8,9]. Here we consider the Szeged index of such graphs. In the next section, we establish a formula for Sz of Cartesian product graphs in terms of their factors and extract some important special cases. This formula, compared with the respective expression for W, indicates that in the case of Cartesian product graphs, Sz exceeds W. In Section 3, we show that a more general result holds, namely that for all (connected) graphs, $Sz \geq W$. We further propose a conjecture about the maximum value of Sz. Finally, in Section 4, we consider the Szeged index of some other composite graphs.

2. THE FORMULA FOR CARTESIAN PRODUCTS

THEOREM 2.1. *For any graphs G and H, $Sz(G \times H) = |G|^3 Sz(H) + |H|^3 Sz(G)$.*

PROOF. Let $P = G \times H$. Since there are only two types of edges in P—corresponding to copies of H and of G, respectively—the Szeged index of P can be written as the sum of

$$\sum_{a \in V(G)} \sum_{xy \in E(H)} n_1((a,x)(a,y) \mid P) \cdot n_2((a,x)(a,y) \mid P),$$

and

$$\sum_{x \in V(H)} \sum_{ab \in E(G)} n_1((a,x)(b,x) \mid P) \cdot n_2((a,x)(b,x) \mid P).$$

Observe now that $n_1((a,x)(a,y) \mid P) = |G| \cdot n_1(xy \mid H)$ and $n_2((a,x)(a,y) \mid P) = |G| \cdot n_2(xy \mid H)$. Analogous statements hold for the edges in copies of G, i.e., edges $(a,x)(b,x)$. Thus, $Sz(P)$ is equal to

$$|G|^3 \sum_{xy \in E(H)} n_1(xy \mid H) \cdot n_2(xy \mid H) + |H|^3 \sum_{ab \in E(G)} n_1(ab \mid G) \cdot n_2(ab \mid G),$$

which completes the proof.

Since the Cartesian product is associative, repeated application of Theorem 2.1 yields the following corollary.

COROLLARY 2.2. *Let $n \geq 2$. Then, for any graphs $G_1, \dots, G_n$ on at least two vertices,*

$$Sz(G_1 \times G_2 \times \cdots \times G_n) = \sum_{i=1}^{n} \left(Sz(G_i) \cdot \prod_{j \neq i} |G_j|^3 \right).$$

Recall from [8,9] that the Wiener index of the Cartesian product of two graphs is given by the formula $W(G \times H) = |G|^2 W(H) + |H|^2 W(G)$, and therefore,

$$W(G_1 \times G_2 \times \cdots \times G_n) = \sum_{i=1}^{n} \left(W(G_i) \cdot \prod_{j \neq i} |G_j|^2 \right).$$

We give two examples for the above results.

(i) Denote the Cartesian product of n copies of a graph G by G^n. Then we have $Sz(G^n) = n|G|^{3(n-1)}Sz(G)$ and $W(G^n) = n|G|^{2(n-1)}W(G)$. The later formula also appears in [8].

(ii) Grid graphs are Cartesian products of paths, i.e., graphs of the form $P_n \times P_m$. Recall from [8,9] that $W(P_n) = 1/6n(n^2-1)$. Since in addition $Sz(P_n) = W(P_n)$, we have $Sz(P_n \times P_m) = 1/6(2n^3m^3 - nm(n^2-m^2))$ which should be compared with $W(P_n \times P_m) = 1/6(n^2m^2(n+m) - nm(n-m))$.

3. RELATION BETWEEN SZEGED AND WIENER INDICES

Comparing the formulas for the Szeged and Wiener index of $G \times H$, it is readily seen that Sz increases with the size of the graphs G and H faster than W. In particular, $Sz(G \times H)$ will exceed $W(G \times H)$ whenever $Sz(G)$ and $Sz(H)$ exceed $W(G)$ and $W(H)$, respectively. This observation is, however, just the tip of an iceberg. Namely, we now demonstrate the following result conjectured in [2].

THEOREM 3.1. *$Sz(G) \geq W(G)$ holds for all (connected) graphs.*

The class of graphs for which Sz and W coincide was characterized by Dobrynin and one of the present authors [4]: these are the graphs with complete blocks. This, in particular, implies that $Sz = W$ for trees and for complete graphs.

Theorem 3.1 could be obtained by combining certain results from [3,4] (but it was not stated in either of those articles. Here we offer a direct and more transparent proof.

Consider a graph G and choose one of the shortest path between each pair of its vertices. The set of these paths is denoted by Ω; its cardinality is $|G|(|G|-1)/2$. (The way in which the elements of Ω are chosen is immaterial.) Let $e = uv$ be an edge of G. Denote by $\Omega(e)$ the subset of Ω containing paths that go through the edge e.

LEMMA 3.2. $W(G) = \sum_{e \in E(G)} |\Omega(e)|$.

PROOF. The right-hand side of the equation counts the distances between all pairs of vertices of G by counting how many times an edge is contained in the (chosen) shortest paths, and then summing the result over all edges. Hence, the lemma.

Denote by x_1 and x_2 the endpoints of the path ω in $\Omega(e)$. If by starting from x_1 and going along ω, the vertex u is passed before v, then x_1 is said to be the u-endpoint, and x_2 the v-endpoint of ω.

Let $N_1^*(e \mid \Omega)$ and $N_2^*(e \mid \Omega)$ be the sets of u-endpoints and v-endpoints, respectively, of the paths from $\Omega(e)$.

Because ω is a shortest path, $x_i \in N_i(e \mid G)$, i.e., $N_i^*(e \mid \Omega) \subseteq N_i(e \mid G)$ for $i = 1,2$. Consequently,

$$|N_i^*(e \mid \Omega)| \leq n_i(e \mid G); \qquad i = 1,2. \tag{1}$$

LEMMA 3.3. $|\Omega(e)| \leq |N_1^*(e \mid \Omega)|\,|N_2^*(e \mid \Omega)|$.

PROOF. Observe that $|\Omega(e)| = |N_1^*(e \mid \Omega)|\,|N_2^*(e \mid \Omega)|$ would hold only if for every pair of vertices x_1 and x_2, $x_1 \in N_1^*(e \mid \Omega)$, $x_2 \in N_2^*(e \mid \Omega)$, there would be a path in $\Omega(e)$, connecting x_1 and x_2. Because not all such paths need to be present in $\Omega(e)$, the inequality follows.

PROOF OF THEOREM 3.1. Combine Lemmas 3.2. and 3.3. with (1).

Among (connected) graphs on n vertices, the path P_n has maximum Wiener index and $W(P_n) = n(n^2-1)/6$ [1]. Thus, the Wiener index increases at most as a third-degree polynomial of the number of vertices.

The Szeged index can increase as a fourth-degree polynomial of the number of vertices. An example for this is the graph $G_n = K_{\lfloor n/2 \rfloor, \lfloor n+1/2 \rfloor}$, for which $Sz(G_n) = n^4/16$, if n is even and $Sz(G_n) = (n+1)^2(n-1)^2/16$ if n is odd.

CONJECTURE. *$K_{\lfloor n/2\rfloor,\lfloor n+1/2\rfloor}$ has maximum Szeged index among all (connected) graphs on n vertices.*

It is known [2] that the conjecture is true for bipartite graphs.

4. NOTE ON THE SZEGED INDICES OF OTHER COMPOSITE GRAPHS

Besides Cartesian product graphs, several other composite graphs were examined in [9]: the join of graphs, the composition of graphs, the corona of graphs and the cluster of graphs. For all of them, formulas are given for the Wiener index of a composite graph in terms of parameters of factors, more precisely in the numbers of edges and vertices of the factors. Although it is also possible to obtain such formulas for the Szeged index of all these compositions, the obtained expressions are not as nice as in the case of the Wiener index. Therefore, we will not write them all down, instead we will present two typical examples. But first, we have to define the corresponding compositions.

The *join* $G+H$ of graphs G and H is obtained from the disjoint union of the graphs G and H, where each vertex of G is adjacent to each vertex of H. The *composition* $G[H]$ of graphs G and H has the vertex set $V(G[H]) = V(G) \times V(H)$ and $(a,x)(b,y)$ is an edge of $G[H]$ if $a = b$ and $xy \in E(H)$, or $ab \in E(G)$. The composition is also known as the *lexicographic product* of graphs.

For brevity, we introduce the following notion. For an edge uv of a graph G, let $N_G(uv)$ be the set of common neighbors of u and v.

We first consider the join $P = G+H$ of graphs G and H. Then $Sz(P)$ is clearly equal to

$$\sum_{ab\in E(G)} n_1(ab \mid P)\cdot n_2(ab \mid P) + \sum_{xy\in E(H)} n_1(xy \mid P)\cdot n_2(xy \mid P) + \sum_{\substack{a\in V(G)\\ x\in V(H)}} n_1(ax \mid P)\cdot n_2(ax \mid P).$$

Since the join of two graphs has diameter at most two, $Sz(P)$ is equal to

$$\sum_{ab\in E(G)} (d_G(a) - |N_G(ab)|)\cdot(d_G(b) - |N_G(ab)|)$$
$$+ \sum_{xy\in E(H)} (d_H(x) - |N_H(xy)|)\cdot(d_H(y) - |N_H(xy)|) + \sum_{\substack{a\in V(G)\\ x\in V(H)}} (|H| - d_H(x))\cdot(|G| - d_G(a)).$$

Comparing this expression with the respective formula for the Wiener index

$$W(G+H) = |G|^2 + |H|^2 + |G|\,|H| - (|G| + |H| + |E(G)| + |E(H)|),$$

we indeed see that the situation is nicer for the Wiener than the Szeged index. However, the formula for the Szeged index becomes more readable in some special cases. For instance, suppose that the graphs G and H are k-regular, triangle-free graphs. Then, for any edge ab of G, we have $|N_G(ab)| = 0$ (and analogously for any edge of H). Thus, we have

$$Sz(G+H) = k^2|E(G)| + k^2|E(H)| + |G|\,|H|(|H| - k)(|G| - k).$$

Similar arguing applies also to the composition of graphs G and H. Without going into details, we state that the Szeged index of $G[H]$ is equal to

$$|G| \sum_{xy\in E(H)} (d_H(x) - |N_H(xy)|)\cdot(d_H(y) - |N_H(xy)|)$$
$$+ \sum_{ab\in E(G)} \sum_{\substack{x\in V(H)\\ y\in V(H)}} (|H| - d_H(y) + |H|n_1(ab \mid G))\cdot(|H| - d_H(x) + |H|n_2(ab \mid G)).$$

REFERENCES

1. I. Gutman, Y.N. Yeh, S.L. Lee and Y.L. Luo, Some recent results in the theory of the Wiener number, *Indian J. Chem.* **32A**, 651–661 (1993).
2. I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, *Graph Theory Notes,* New York **27**, 9–15 (1994).
3. A. Dobrynin and I. Gutman, On a graph invariant related to the sum of all distances in a graph, *Publ. Inst. Math. (Beograd)* **56**, 18–22 (1994).
4. A. Dobrynin and I. Gutman, Solving a problem connected with distances in graphs, *Graph Theory Notes,* New York **28**, 21–23 (1995).
5. A.A. Dobrynin, I. Gutman and G. Dömötör, A Wiener-type graph invariant for some bipartite graphs, *Appl. Math. Lett.* **8** (5), 57–62 (1995).
6. I. Gutman, P.V. Khadikar, P.V. Rajput and S. Karmarkar, The Szeged index of polyacenes, *J. Serb. Chem. Soc.* **60**, 759–764 (1995).
7. P.V. Khadikar, S. Karmarkar, S. Joshi and I. Gutman, Estimation of protonation constants of salicylhydroxamic acids by means of the Wiener topological index, *J. Serb. Chem. Soc.* (to appear).
8. A. Graovac, and T. Pisanski, On the Wiener index of a graph, *J. Math. Chem.* **8**, 53–62 (1991).
9. Y.N. Yeh and I. Gutman, On the sum of all distances in composite graphs, *Discrete Math.* **135**, 359–365 (1994).