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SOME GRAPHS WITH EXTREMAL SZEGED INDEX

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ABSTRACT. Szeged index of a graph is a graph invariant which "measures" some distance properties of graphs (which are significant in mathematical chemistry). In this paper we identify, among bicyclic and tricyclic graphs, those graphs whose Szeged index is extremal (minimal and maximal).

1. Introduction

All graphs considered in this paper are simple graphs, i.e. undirected graphs without loops or multiple edges. The sum of distances between all pairs of vertices of a (connected) graph is an invariant that has been extensively studied in the mathematical literature (see, for instance [6], [10] and the references cited therein; an entire issue of *Discrete Applied Mathematics* — to appear in 1997 will be devoted to the 50th anniversary of this quantity). In chemistry this invariant is also known as Wiener index, or Wiener number; for further details see [7].

For a connected graph $G = (V, E)$ its Wiener index (denoted by $W(G)$) is defined as follows:

$$W(G) = \sum_{\{x,y\} \subseteq V} d(x, y; G),$$

where $d(x, y; G)$ denotes the distance between the vertices x and y in the graph G (see, for example, [1] for other details). In this paper we focus our attention to an invariant closely related to $W(G)$, which was recently introduced in [5] and eventually named the *Szeged index* ([8]). As a proper consequence of its definition, the Szeged index coincides with the Wiener index at least for trees. For more details, including motivational and historical discussions, the reader is referred to [5].

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Assume now that $G = (V, E)$ is a connected graph and $e = \{u, v\}$ is its edge. Define two sets $N_u(e)$ and $N_v(e)$ with respect to e as follows:

$$N_u(e) = \{x \in V : \ d(u, x; G) < d(v, x; G)\} ,$$
$$N_v(e) = \{x \in V : \ d(v, x; G) < d(u, x; G)\} .$$

Clearly, $u \in N_u(e)$, while $v \in N_v(e)$. These two sets are disjoint, and in general, do not include all vertices of G. If G is connected and if e does not belong to an odd-cycle, then these sets induce a bisection of the vertex set of G.

Let $n_u(e) = |N_u(e)|$, $n_v(e) = |N_v(e)|$; in other words, $n_u(e)$ (resp. $n_v(e)$) is the number of vertices of G which are closer to u than v (resp. closer to v than u). Note that the vertices equidistant to u and v, or not reachable from u and v are not counted. For any (not necessarily connected) graph G with at least two vertices, its Szeged index (denoted by $\mathrm{Sz}(G)$) is defined as follows:

$$\mathrm{Sz}(G) = \sum_{e \in E} \pi(e) ,$$

where

$$\pi(e) = n_u(e)\, n_v(e) \qquad (e = \{u, v\}) .$$

For the purpose of the subsequent discussion we also define

$$\sigma(e) = n_u(e) + n_v(e) ,$$
$$\delta(e) = |n_u(e) - n_v(e)| .$$

According to [5], from the above definitions, we easily get

$$\pi(e) = \sum_{\{x,y\} \subseteq V} \mu_{x,y}(e) , \tag{1}$$

where $\mu_{x,y}(e)$, interpreted as the contribution of the vertex pair x, y to the above product (or generally to Szeged index) is defined as follows (recall that $e = \{u, v\}$):

$$\mu_{x,y}(e) = \begin{cases} 1 & \text{if } \begin{cases} d(x,u) < d(x,v) \text{ and } d(y,v) < d(y,u) , \\ \text{or} \\ d(x,v) < d(x,u) \text{ and } d(y,u) < d(y,v) , \end{cases} \\ 0 & \text{otherwise.} \end{cases}$$

Observe that the summation in (1) goes over all 2-element subsets $\{x, y\}$ of V. (Notice also some formal difference between this definition and the one from [5].)

It is worth noting that $\mathrm{Sz}(G) = W(G)$ if G is a tree. Generally, we have

$$\mathrm{Sz}(G) \geq W(G) ,$$

with equality (settled in [4]) if and only if all blocks of G are complete graphs. In Section 2 we prove the above inequality (Theorem 2.1) and offer an alternative proof of the equality case. In Section 3 (Section 4) we find all bicyclic and tricyclic graphs for which the Szeged index is minimal (resp. maximal).

2. Some preliminary results

We first prove:

THEOREM 2.1. *For every connected graph G (with at least two vertices),*

$$\mathrm{Sz}(G) \geq W(G)\,, \tag{2}$$

with equality if and only if each block of G is a complete graph.

P r o o f. Assume $G = (V, E)$. Then we have

$$\sum_{e \in E} \mu_{x,y}(e) \geq d(x, y; G)\,, \tag{3}$$

for any $x, y \in V$. To see this take a shortest path between x and y. Then $\mu_{x,y}(e) = 1$ whenever e belongs to this path. From (3), by summing over all 2-vertex subsets $\{x, y\}$ $(x, y \in V)$, we get (2).

Clearly, the equality in (2) holds if and only if equality in (3) holds for each subset $\{x, y\}$. To complete the proof, suppose that some block (of G), say B, is not a complete graph (note that this also implies that B has at least four vertices). Since in general any two vertices belonging to a (nontrivial) block belong to a cycle (also contained in the block), we consider the shortest such cycle embracing two nonadjacent vertices (say x and y). The vertices of this cycle induce a subgraph of B, isomorphic either to a cycle C_n $(n \geq 4)$, or to the graph $C_4 + c$, where c is a chord. With these assumptions, $\mu_{x,y}(e) = 1$ for any edge e $(\neq c)$ belonging to the considered graphs. Consequently, equality in (3) does not hold in this particular case. On the other hand, if all blocks of G are complete graphs, then (3) is always satisfied with equality. □

Note that Theorem 2.1 was deduced in [9], by employing another way of reasoning.

In what follows, we shall be concerned with finding those (connected) (n, m)-graphs (on n vertices and with m edges) for which the Szeged index is extremal. For trees $(m - n - 1)$ and unicyclic graphs $(m = n)$ we can easily identify the corresponding graphs (see also [5]). To make the paper self-contained we state the corresponding results.

THEOREM 2.2. *For any tree G (on n vertices), other than $K_{1,n-1}$ and P_n, we have*

$$\mathrm{Sz}(K_{1,n-1}) < \mathrm{Sz}(G) < \mathrm{Sz}(P_n) .$$

For convenience, let

$$U_n = \begin{cases} C_n , & n \text{ is even,} \\ C_{n-1} \cdot K_2 , & n \text{ is odd.} \end{cases}$$

(Here $\cdot$ stands for a dot product of corresponding graphs.)

THEOREM 2.3. *For any connected unicyclic graph G (on n vertices), other than $K_{1,n-1} + e$ and U_n, we have*

$$\mathrm{Sz}(K_{1,n-1} + e) < \mathrm{Sz}(G) < \mathrm{Sz}(U_n) .$$

In the next two sections we extend the above results, among others, to bicyclic graphs ($m = n + 1$) and tricyclic graphs ($m = n + 2$).

3. Graphs with minimal Szeged index

We first give a sharp lower bound for the Szeged index of any (n, m)-graph.

LEMMA 3.1. *If G is a connected (n,m)-graph, then*

$$\mathrm{Sz}(G) \geq 2\binom{n}{2} - m . \tag{4}$$

P r o o f . By (2) we have $\mathrm{Sz}(G) \geq W(G)$. Since

$$\min W(G) = m + 2\left[\binom{n}{2} - m\right] ,$$

we are done. (Note that all distances between nonadjacent vertices are truncated to 2.) □

Now the question is whether the bound from (4) is attained. Generally, the answer depends on m (for fixed n) and in many cases it is positive. The bound is attained if (and only if) there exists a graph H such that $\mathrm{Sz}(H) = W(H)$ and $W(H) = 2\binom{n}{2} - m$. In particular, for bicyclic and tricyclic graphs we have the following results. (Proofs are omitted since being obvious.)

THEOREM 3.2. *For any bicyclic graph G (on n vertices), other than $K_{1,n-1} + e + f$ (edges e and f induce $2K_2$), we have*

$$\mathrm{Sz}(G) > \mathrm{Sz}(K_{1,n-1} + e + f) .$$

THEOREM 3.3. *For any tricyclic graph G (on n vertices), other than $K_{1,n-1}+e+f+g$ (edges e, f and g induce either K_3, or $3K_2$), we have*

$$\mathrm{Sz}(G) > \mathrm{Sz}(K_{1,n-1}+e+f+g)\,.$$

Note, for tricyclic graphs we have identified two graphs with minimal Szeged index. In the general case the situation may become messy, and also (4) need not be attained. For fixed n and m, (4) is satisfied if there exists a graph H whose all blocks are complete graphs, and whose diameter is 2 (what in turn implies that all blocks have a fixed vertex in common). The latter is equivalent to partitioning $n-1$ (into, say k, summands $n_1, n_2, \ldots, n_k$), such that

$$\binom{n_1}{2}+\binom{n_2}{2}+\cdots+\binom{n_k}{2}=m-(n-1)\,.$$

However, for some values of m (e.g. $m > \binom{n-1}{2}$; n being fixed) this is not possible.

4. Graphs with maximal Szeged index

Let G be an arbitrary (n,m)-graph. Then we have

$$\mathrm{Sz}(G) \le m \max_{e\in E} \pi(e)\,.$$

Since $\pi(e) \le \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$, we get the following bound

$$\mathrm{Sz}(G) \le f(n,m)\ \left(= m\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil\right). \tag{5}$$

Throughout the paper $\lfloor x \rfloor$ is the greatest integer $\le x$, while $\lceil x \rceil$ is the least integer $\ge x$. This bound is attained if and only if for each edge e the following two conditions are satisfied:

$$\sigma(e) = n\,, \tag{6}$$

and

$$\delta(e) \le 1\,. \tag{7}$$

On the other hand, if for some edge e, either (6) or (7) does not hold, the following applies:

a) If (6) does not hold, then

$$\pi(e) \le \left\lfloor \frac{n}{2} \right\rfloor \left(\left\lceil \frac{n}{2} \right\rceil - 1\right),$$

so $\mathrm{Sz}(G)$ is reduced by at least $\lfloor \frac{n}{2} \rfloor$ for any such edge.

b) If (7) does not hold, then

$$\pi(e) \le \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil - \phi(e)\,,$$

where

$$\phi(e) = \begin{cases} \frac{1}{4}\delta^2(e)\,, & n \text{ is even,} \\ \frac{1}{4}\big(\delta^2(e) - 1\big)\,, & n \text{ is odd.} \end{cases}$$

Now $\mathrm{Sz}(G)$ is reduced by at least $\phi(e)$ for any such edge.

Based on these observations, we shall in sequel say that an edge e is

- *good* if $\pi(e) = \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$ (both (6) and (7) hold, whereas $0 \le \delta(e) \le 1$);
- *almost good* if $\pi(e) = \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil - 1$ for n even, or $\pi(e) = \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil - 2$ for n odd ((6) holds, but not (7), whereas $2 \le \delta(e) \le 3$);
- *bad* otherwise.

In the next two lemmas, let G (if it exists) be an (n,m)-graph whose all edges are good, except s (≥ 0) which are almost good. Any such graph is, of course, a good candidate (within the class of (n,m)-graphs) to have the largest Szeged index. As we see soon, such graphs (for n large enough) do exist at least in the class of bicyclic and tricyclic graphs. Moreover, they turn to be bipartite since (6) always holds (essential for Lemma 4.2).

LEMMA 4.1. *Let G be a graph as above, and H an (n,m)-graph having at least one pendant edge. Then*

$$\mathrm{Sz}(G) > \mathrm{Sz}(H)$$

whenever $n > \sqrt{8s+1} + 2$ for n odd, or $n > 2\big(\sqrt{s} + 1\big)$ for n even.

Proof. Under the above assumptions, for odd n $(= 2k+1)$ we have

$$\mathrm{Sz}(H) \le (m-1)k(k+1) + 2k < (m-s)k(k+1) + s(k-1)(k+2) = \mathrm{Sz}(G)\,,$$

whereas for even n $(= 2k)$,

$$\mathrm{Sz}(H) \le (m-1)k^2 + 2k - 1 < (m-s)k^2 + s(k-1)(k+1) = \mathrm{Sz}(G)\,.$$

Thus $\mathrm{Sz}(H) < \mathrm{Sz}(G)$ holds, as required. □

LEMMA 4.2. *Let G be a (bipartite) graph as above, and H a nonbipartite (n,m)-graph. Then*

$$\mathrm{Sz}(G) > \mathrm{Sz}(H)$$

whenever $n > \frac{2}{3}s$ for n even, or $n > \frac{4}{3}s + 1$ for n odd

Proof. Let C be the shortest odd-cycle of H (g denoting its length). Further, let u, v be two vertices of C, and let $d(u,v;C)$ be their distance in C (C is regarded as an induced subgraph of H). Then, clearly, $d(u,v;H) \le$

$d(u,v;C)$. Next suppose that $d(u,v;H) < d(u,v;C)$. Let $P(u,v;H)$, $P(u,v;C)$ be the corresponding shortest paths. If $d(u,v;H)$ and $d(u,v;C)$ are of different parity, we get a contradiction — the subgraph induced by the vertices from these paths contains a shorter odd-cycle. Otherwise, observe the complementary path on C, i.e. $P^*(u,v;C)$, and $P(u,v;H)$. Their lengths are of different parity, and hence the same contradiction appears. Thus the distances in question are all equal. So for any edge $e = \{u,v\}$ of C there exists a vertex w on C (equidistant to u and v in C), and as well equidistant to u and v in H. In other words (6) does not hold for e. Thus (see (a)) we get

$$\mathrm{Sz}(H) \le f(n,m) - g\left\lfloor \frac{n}{2} \right\rfloor ,$$

since each edge e (belonging to C) reduces the Szeged index by $\lfloor \frac{n}{2} \rfloor$.

On the other hand

$$\mathrm{Sz}(G) = f(n,m) - \begin{cases} s\,, & n \text{ is even,} \\ 2s\,, & n \text{ is odd.} \end{cases}$$

But now, since $g \ge 3$, we are done. □

We also need the following general lemma (holding for any graph G).

Lemma 4.3. *Given an edge $e = \{u,v\}$ of some graph G, let $N_u(e)$ and $N_v(e)$ be defined as in Section 1. If the vertices $x \in N_u(e)$ and $y \in N_v(e)$ are adjacent then $d(u,x;G) = d(v,y;G)$.*

P r o o f. Without loss of generality, assume $d(u,x;G) < d(v,y;G)$. But then $d(u,y;G) \le d(u,x;G) + d(x,y;G) \le d(v,y;G)$ since $d(x,y;G) = 1$. Thus we get a contradiction, i.e., $y \notin N_v(e)$. □

The next lemma refers to Θ-graphs. Recall that a graph is a Θ*-graph* if it consists of at least three (parallel) paths connecting two fixed vertices (alternatively, it is homeomorphic to a multigraph on two vertices having at least three multiple edges).

Lemma 4.4. *Let $G = (V,E)$ be a Θ-graph having k (≥ 3) (parallel) paths. Then an edge e (of G) is good if and only if*

- *G is bipartite (hence the lengths of all paths are of same parity);*
- *e is placed in the middle position of some path, unless $k = 3$ and n even, when two exceptions are possible (see the proof).*

P r o o f. If G is nonbipartite, then each edge of G (since it is a Θ-graph) belongs to some odd-cycle and hence none of them is good. Otherwise, each cycle is even and (6) always holds.

Assume now that x and y are vertices in G of degrees greater than 2, and that $e = \{u, v\}$ belongs to $P^{(i)}$, the i-th path connecting x and y. Then, with respect to $N_u(e)$ and $N_v(e)$, we can have:

- x and y are in different sets;
- x and y are in the same set.

In the first case we claim that

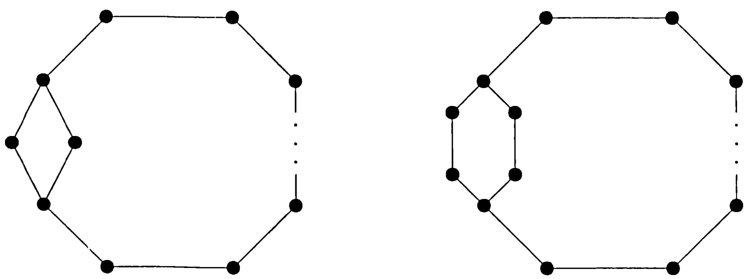
$$\delta(e) = (k-2)|b_i - a_i|, \tag{8}$$

where a_i (b_i) is the distance between x (resp. y) and the edge e. To see this, observe on $P^{(j)}$ ($j \neq i$) two adjacent vertices u_j and v_j such that $u_j \in N_u(e)$ and $v_j \in N_v(e)$. By Lemma 4.3, $d(u, u_j; G) = d(v, v_j; G)$ holds, and thus on each path $P^{(j)}$ ($j \neq i$) we shall have $b_i - a_i$ vertices more in $N_u(e)$ than in $N_v(e)$. Hence $|N_u(e)| - |N_v(e)| = (k-1)(b_i - a_i) + (a_i - b_i)$, what gives (8). Consequently, e is good if and only if either $b_i = a_i$, or otherwise if $k = 3$ and $|b_i - a_i| = 1$ (the first exception).

In the second case we claim that

$$\delta(e) = |V(G)| - g, \tag{9}$$

where g is the length of the shortest cycle (of G) containing e.



B_n (n odd) B_n (n even)

FIGURE 1.

To see this, assume (without loss of generality) that $x, y \in N_v(e)$. But then all vertices from paths $P^{(j)}$ ($j \neq i$) are in $N_v(e)$, and hence $|N_u(e)| = \frac{g}{2}$ (note that g is even), while $|N_v(e)| = |V(G)| - \frac{g}{2}$, what implies (9). Therefrom, by simple arguments, we get that $\delta(e) \leq 1$ if and only if e is an arbitrary edge of B_n (see Fig. 1 for n odd and $n \geq 7$) not belonging to cycle of length four (the second exception, which also appears for $k = 3$). □

In the remaining part of the paper we focus our attention to bicyclic and tricyclic graphs.

THEOREM 4.5. *If G_n is a bicyclic graph on $n > 6$ vertices other than B_n, then*

$$\mathrm{Sz}(G_n) < \mathrm{Sz}(B_n).$$

Proof. We first note that all edges of B_n are good if n is odd, while only three such edges are good if n is even (others are almost good) — see Lemma 4.4. Consider now any bicyclic graph G_n (on n vertices) other than B_n.

Assume first that G_n has at least one pendant edge. But then, by Lemma 4.1, even for $n > 6$ we are done ($\mathrm{Sz}(G_n) < \mathrm{Sz}(B_n)$). So assume next that G_n is homeomorphic to one of the three bicyclic graphs without pendant edges — two of them are 1-connected, while one (a Θ-graph) is 2-connected. In addition, in view of Lemma 4.2, assume that G_n is bipartite.

If G_n is 1-connected, then it consists of two disjoint cycles (linked by a path), or two cycles with a common vertex. But then none of the edges taken from the cycles is good. On the other hand, at most two edges belonging to the (linking) path can be good. Since B_n has at least three good edges, we are done.

If G_n is 2-connected, then it is a Θ-graph. Let $a \le b \le c$ be the lengths of the corresponding paths (which are of the same parity since G_n is bipartite).

Assume first that n is odd. Then a, b, c are all even ($a + b + c = n + 1$). Suppose that $b \ge 4$, and let x be an edge belonging to this path, incident to a vertex of degree 3. By Lemma 4.4 (see (8) or (9)) we get $\delta(x) \ge 3$. So x is not good (recall that all edges of B_n are good), and thus $\mathrm{Sz}(G_n) < \mathrm{Sz}(B_n)$.

Otherwise, if $b = 2$, then $a = 2$ as well, and hence we get B_n.

We now assume that n is even. Hence a, b, c are all odd. If $b \ge 5$, as above, let x be an edge belonging to this path, incident to a vertex of degree 3. By Lemma 4.4 (as above), we now get $\delta(x) \ge 4$. Consequently, x is bad and thus $\mathrm{Sz}(G_n) < \mathrm{Sz}(B_n)$. (Recall that B_n has no bad edges, while having three good edges, i.e. the maximal possible number.)

Next assume $b = 3$. If so, then $a = 1$, or $a = 3$. If $a = 1$, then x is again bad ($\delta(x) = n - 4$) whenever $n \ge 8$. So, again, $\mathrm{Sz}(G_n) < \mathrm{Sz}(B_n)$. If, on the other hand, $a = 3$, then we get B_n, as required. □

THEOREM 4.6. *If G_n is a tricyclic graph on $n \ge 12$ vertices other than T_n (see Fig. 2), then*

$$\mathrm{Sz}(G_n) < \mathrm{Sz}(T_n).$$

(The expressions appearing in Fig. 2 stand for the number of vertices.)

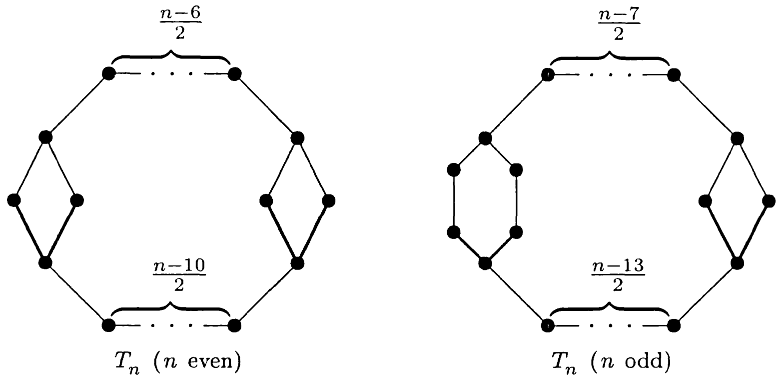


FIGURE 2.

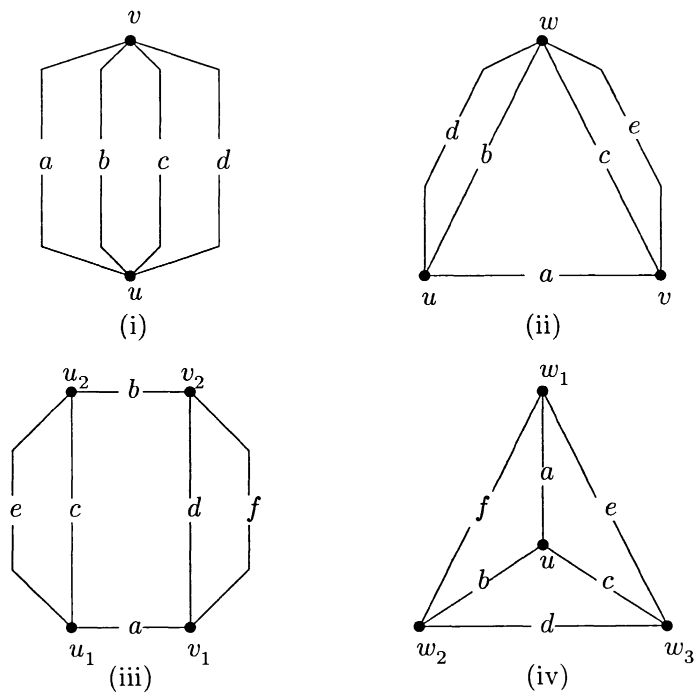


FIGURE 3.

P r o o f. We first note that all edges of T_n are good except s $(= 4)$ edges which are almost good — the heavy edges in Fig. 2. So

$$\mathrm{Sz}(T_n) = f(n, n+2) - \begin{cases} s\,, & n \text{ is even,} \\ 2s\,, & n \text{ is odd.} \end{cases}$$

Consider now any tricyclic graph G_n (on n vertices), other than T_n. If there exists a pendant edge in G_n, then $\mathrm{Sz}(G_n) < \mathrm{Sz}(T_n)$ (by Lemma 4.1 since $n \geq 12$ and $s = 4$). Thus in what follows we may assume that G_n is homeomorphic to one of the 15 tricyclic graphs without pendant edges. Note that 11 among these graphs are 1-connected, while 4 are 2-connected, i.e., blocks (see Fig. 3). In addition, in view of Lemma 4.2, we can also take that G_n is bipartite.

Since $s = 4$ is rather small, we reject from further considerations those graphs G_n that have more than one bad edge, or those with one bad edge, say e, if

- $4 \leq \delta(e) \leq 5$ and at least one edge (for n even) or two edges (for odd n) exist which are not good,

or

- $\delta(e) \geq 6$.

We first assume that G_n is 1-connected. If so, then G_n can be represented as a "dot product" of some bicyclic graph B $(= (V(B), E(B)))$ and a cycle C. Since $\delta(e) \geq |V(B)| - 1 \geq 4$, all edges of C are bad. Thus $\mathrm{Sz}(G_n) < \mathrm{Sz}(T_n)$.

Let, therefore, G_n be 2-connected. Then it is equal to one of the graphs (blocks) depicted in Fig. 3. The letters $a, b, \ldots, f$ stand for the lengths of the corresponding paths between vertices of degree greater than 2. For the sake of brevity, we refer to these paths as $P(a), P(b), \ldots, P(f)$, respectively.

In order to complete the proof, we consider the following four cases:

Case 1: G_n is the graph on Fig. 3(i).
Then G_n is a Θ-graph with $k = 4$. By Lemma 4.4, G_n could have at most 4 good edges (see the proof). On the other hand, for each $n \geq 12$, T_n has $n - 2$ good edges. So $\mathrm{Sz}(G_n) < \mathrm{Sz}(T_n)$.

Case 2: G_n is the graph on Fig. 3(ii).
Without loss of generality, let $d \geq b$, $e \geq c$. Assume first that $d > b$ (thus $d \geq b + 2$, since G_n is bipartite), and let x be the edge belonging to $P(d)$, and incident to u. Then

$$\delta(x) = \begin{cases} a + c + e - 2, & b \leq a + c, \\ b + e - 2, & b \geq a + c. \end{cases}$$

Therefrom we get

$$\delta(x) \geq a + c + e - 2.$$

Similarly,

$$\delta(x') \geq a + c + e - 2,$$

where x' is the edge from the same path, but incident to w (note $x \neq x'$ since $d \geq 3$). But now, if $a \geq 2$, or $c + e \geq 6$ (this sum must be even), then both edges x and x' are bad. So we have $\mathrm{Sz}(G_n) < \mathrm{Sz}(T_n)$. Otherwise, assume $a = 1$ and $c + e = 4$. If $e = 3$ and $c = 1$, then (by the same argument), we also get b d 4, and thus $n = a + b + c + d + e - 2 < 12$. So assume $c = e = 2$.

If $b \geq 4$ then $\delta(x) \geq 4$ (since $b \geq a+c$). But then $\delta(x') \geq 4$ as well, and we are done. Otherwise, let $b = 1$, or $b = 3$ (note that b must be odd). If $b = 1$, then take $y = \{u, v\}$. Now $\delta(y) = n - 3 \geq 9$, and we have $\mathrm{Sz}(G_n) < \mathrm{Sz}(T_n)$. If $b = 3$, then it is easy to find at least five edges in G_n which are almost good (two on $P(b)$ incident to u or v, and three on $P(d)$, two of which are incident to u or v). Hence, if $b \neq d$ or $c \neq e$ we are done.

In what remains let $d = b$, $e = c$, and assume also, without loss of generality, that $b \geq c$. Further, let x be the edge belonging to $P(c)$ and incident to w. Then

$$\delta(x) = \begin{cases} b+c-2\,, & a \geq b-c\,, \\ a+2c-2\,, & a \leq b-c\,. \end{cases}$$

If $c \geq 3$, then $b \geq 3$ as well, and therefore $\delta(x) \geq 4$. Since another bad edge appears on $P(e)$, we get $\mathrm{Sz}(G_n) < \mathrm{Sz}(T_n)$. Next assume that $c = 2$. Then $a + 2b \geq 10$ (recall $n \geq 12$). If $a \geq 2$ and $b \geq 4$, then $\delta(x) \geq 4$, and thus $\mathrm{Sz}(G_n) < \mathrm{Sz}(T_n)$. If $a = 1$ and $b \geq 5$, then both edges belonging to $P(b)$ (or $P(d)$), incident to w are bad ($\delta(y) = b$, where y is any of these edges). Consequently, we have $\mathrm{Sz}(G_n) < \mathrm{Sz}(T_n)$. Finally, if $b = 2$ and $a \geq 6$, or $b = 3$ and $a \geq 4$, G_n has no bad edges, but then we can find in it at least five almost good edges (for instance, four edges incident to w are almost good, and also each of two edges on $P(a)$, incident to u or v). So we are done.

Case 3: G_n is the graph on Fig. 3(iii).
Without loss of generality, let $e \geq c$, $f \geq d$. Assume first that $e > c$ (thus $e \geq c+2$ since G_n is bipartite). Let x be an edge belonging to $P(e)$, incident to u_1. Then

$$\delta(x) = \begin{cases} a+b+d+f-2\,, & c \leq a+b+d\,, \\ c+f-2\,, & c \geq a+b+d\,. \end{cases}$$

Therefrom we get

$$\delta(x) \geq (a+b) + (d+f) - 2 \geq 4\,.$$

Hence x is bad. Since there exists another bad edge on the same path (like x' from Case 2), we have $\mathrm{Sz}(G_n) < \mathrm{Sz}(T_n)$. So in what remains we assume that $e = c$ and $d = f$. Without loss of generality, we also assume that $a < b$, $c \geq d$. Let x be an edge on $P(c)$ incident to u_1. If $c \geq 4$ we easily get that x is bad, and since the same holds for x' (chosen as above), we have $\mathrm{Sz}(G_n) < \mathrm{Sz}(T_n)$. Moreover, if $c = 3$ and $d = 3$, then the same argument can be applied. Consequently, $d = 2$. If $c = d = 2$, then x is almost good. Thus, by symmetry, we have now recognized four almost good edges. Consider next an edge belonging to $P(c)$, and incident to u_2. This edge is good if and only if $b - a = 2$. But then we get T_n (with n being even). If $c = 3$ and $d = 2$, then, again, x is almost good. Together with x' (as specified above), we have so far two almost good edges. By taking y and y', edges on $P(d)$ and $P(f)$ incident to v_1 we get two more almost good edges. As in former analysis, consider next an edge belonging to $P(c)$, incident to u_2. This edge is good if and only if $b - a = 3$. But then we get T_n (with n being odd).

Case 4: G_n is the graph on Fig. 3(iv).
Without loss of generality, assume $a = \max\{a, b, c, d, e, f\}$, and $b \geq c$. Let $x = \{u, v\}$ be an edge belonging to $P(a)$. Then $w_i \in N_u(x)$ $(i = 2, 3)$, since $d(u, w_i; G_n) \leq d(v, w_i; G_n)$ by the choice of a. Moreover, equality cannot hold because G_n is bipartite. Next, let $l(x)$ be the length of the shortest cycle (of G_n) containing x. Then $w_1 \in N_u(x)$ if $a > \frac{1}{2}l(x)$, or otherwise, $w_1 \in N_v(x)$ if $a \leq \frac{1}{2}l(x)$.

Assume first $a > \frac{1}{2}l(x)$ $(w_1, w_2, w_3 \in N_u(x))$. Now $N_u(x)$, $N_v(x)$ form a bisection of the vertex set of G_n, with two "cross" edges (one is x, the other is y, also belonging to the same path). By using Lemma 4.3 we easily get

$$\delta(x) = n - l(x)\,.$$

Clearly, we have to consider only the situations where $\delta(x) \leq 3$, since otherwise x (along with x' which belongs to the same path, but being incident to w_1) is bad. On the other hand, we have $\delta(x) \geq 2$ (otherwise, we have to tune the parameters of G_n so that either a triangle inequality is violated, or a triangle appears). Hence, x is almost good. In addition, notice that y (another edge between $N_u(x)$ and $N_v(x)$) is also bad. If y is not incident to w_1, we can "shift" x (and y) along $P(a)$ (according to Fig. 3(iv) upwards) to get another pair, say x_1 and y_1, of bad edges. If neither x_1 nor y_1 is adjacent to w_1 we can do the same once again, but then we already have six bad edges; so we have $\mathrm{Sz}(G_n) < \mathrm{Sz}(T_n)$. Generally, we can obtain $a - \frac{1}{2}l(x)$ pairs of bad edges in this way. So if $a - \frac{1}{2}l(x) \leq 2$, we need some other arguments to reject G_n. We first notice that there are at most 6 vertices of G_n not on $P(a)$ (at most 3 not belonging to the observed cycle, and at most 3 on it — the latter follows owing to the choice of the cycle). So, $l(x) \leq a + 4$, and thus $a \leq 8$. In other words, we have $n \leq 15$. Then this section of the proof is completed by means of a brute force checking (employing, for instance, the computer package GRAPH [2]).

Assume next $a \leq \frac{1}{2}l(x)$ $(w_1 \in N_v(x),\ w_2, w_3 \in N_u(x))$. Now $N_u(x)$, $N_v(x)$ form a bisection of the vertex set of G_n, with three cross edges (one is x, other two being y and z, belonging to $P(e)$ and $P(f)$, respectively). By using Lemma 4.3, we get

$$\delta(x) = \begin{cases} a + d - 2\,, & d \geq |b - c|\,, \\ a + |b - c| - 2\,, & d \leq |b - c|\,. \end{cases}$$

Thus $\delta(x) \geq a + d - 2$, and consequently, if $a \geq 5$, or if $a = 4$ and $d \geq 2$, or even if $a = d = 3$ we have $\delta(x) \geq 4$. If so, then we have $\mathrm{Sz}(G_n) < \mathrm{Sz}(T_n)$ (since x' chosen as above is also bad). In what remains, by symmetry argument, we have $a+d \leq 5$, $b+e \leq 5$ and $c+f \leq 5$, and consequently $n \leq 13$. To reject these possibilities we can again proceed by a brute force checking.

This completes the proof. □

Remark. If $n = 11$, then the graph T_n is still maximal, provided its two cycles have a vertex in common (as in Case 2 from the above theorem). Moreover, for $n = 10$, T_n is maximal. Smaller values of n can be easily checked even by hand.

Added in proof:

In the meantime we have learnt that $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ is the unique graph with maximal Szeged index in the set of all connected graphs with n vertices (see [3]).

REFERENCES

[1] BUCKLEY, F.—HARARY, F.: *Distance in Graphs*, Addison-Wesley, Reading, 1990.

[2] CVETKOVIĆ, D. M.—SIMIĆ, S. K.: *Graph theoretic results obtained by the support of the expert system "GRAPH"*, Bull. Acad. Serbe Sci. Arts Cl. Sci. Math. Natur. **107** (1994), 19–41.

[3] DOBRYNIN, A. A.: *Graphs having the maximal value of the Szeged index*, Croat. Chem. Acta **70** (1997), 819–825.

[4] DOBRYNIN, A.—GUTMAN, I.: *Solving a problem connected with distances in graphs*, Graph Theory Notes New York **28** (1995), 21–23.

[5] GUTMAN, I.: *A formula for the Wiener number of trees and its extension to graphs containing cycles*, Graph Theory Notes New York **27** (1994), 9–15.

[6] GUTMAN, I.—YEH, Y. N.: *The sum of all distances in bipartite graphs*, Math. Slovaca **45** (1995), 327–334.

[7] GUTMAN, I.—YEH, Y. N.—LEE, S. L.—LUO, Y. L.: *Some recent results in the theory of the Wiener number*, Indian J. Chem. **32A** (1993), 651–661.

[8] KHADIKAR, P. V.—DESHPANDE, N. V.—KALE, P. P.—DOBRYNIN, A.—GUTMAN, I.—DÖMÖTÖR, G.: *The Szeged index and an analogy with the Wiener index*, J. Chem. Inf. Comput. Sci. **35** (1995), 547–550.

[9] KLAVŽAR, S.—RAJAPAKSE, A.—GUTMAN, I.: *On the Szeged and the Wiener index of graphs*, Appl. Math. Lett. **9(5)** (1996), 45–49.

[10] YEH, Y. N.—GUTMAN, I.: *On the sum of all distances in composite graphs*, Discrete Math. **135** (1994), 359–365.

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