

COMPLEXITY OF THE SZEGED INDEX, EDGE ORBITS, AND SOME NANOTUBICAL FULLERENES

YASER ALIZADEH

Department of Mathematics, Hakim Sabzevari University, Sabzevar, Iran

e-mail: `y.alizadeh@hsu.ac.ir`

SANDI KLAVŽAR

Faculty of Mathematics and Physics, University of Ljubljana, Slovenia

Faculty of Natural Sciences and Mathematics, University of Maribor, Slovenia

Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenia

e-mail: `sandi.klavzar@fmf.uni-lj.si`

Abstract Let I be a summation-type topological index. The I -complexity $C_I(G)$ of a graph G is the number of different contributions to $I(G)$ in its summation formula. In this paper the complexity $C_{Sz}(G)$ is investigated, where Sz is the well-studied Szeged index. Let $O_e(G)$ (resp. $O_v(G)$) be the number of edge (resp. vertex) orbits of G . While $C_{Sz}(G) \leq O_e(G)$ holds for any graph G , it is shown that for any $m \geq 1$ there exists a vertex-transitive graph G_m with $C_{Sz}(G_m) = O_e(G_m) = m$. Also, for any $1 \leq k \leq m + 1$ there exists a graph $G_{m,k}$ with $C_{Sz}(G_{m,k}) = O_e(G_{m,k}) = m$ and $C_W(G_{m,k}) = O_v(G_{m,k}) = k$. The Sz-complexity is determined for a family of (5,0)-nanotubical fullerenes and the Szeged index is compared with the total eccentricity.

1 Introduction

In mathematical chemistry, any function which assigns a real number to a (chemical) graph and is invariant under graph isomorphism is called a *topological index*. Of course, one has countless possibilities how to define a (new) topological index; hence it is important to design it to be applicable and, also not negligible, mathematically appealing. The reader is invited to books [14, 15, 28] for examples of topological indices that have passed these requirements. We also refer to [12, 25] for a couple of recent chemical applications, to [5] for a recent investigation of several infinite convex benzenoid networks via numerous topological indices, as well as to [17] for studies of additional topological indices on hex-derived networks.

In this paper we are primarily interested in the Szeged index that turned out to be one of the relevant topological indices. It was introduced in [13] and proved to be chemically relevant in [6, 18] as well as in [5], where Szeged-like indices are involved in the investigation. The papers [16, 22] present a couple of recent developments on the Szeged index.

Let $G = (V(G), E(G))$ be a graph. Suppose that a topological index I either of the form

$$I(G) = \sum_{v \in V(G)} f(v), \quad (1)$$

or of the form

$$I(G) = \sum_{e \in E(G)} f(e), \quad (2)$$

where $f : V(G) \rightarrow \mathbb{R}$ (resp. $f : E(G) \rightarrow \mathbb{R}$) is a real function. The most striking example is obtained by setting $f(v)$ to be the sum of the distances from v to all the other vertices, because in this case (1) reads as $I(G) = 2W(G)$, where $W(G)$ is the Wiener index of G . Vertices u and u' (resp. edges e and e') are in relation \sim_I if $f(u) = f(u')$ (resp. $f(e) = f(e')$). Clearly, \sim_I is an equivalence relation. Let $V(G)/\sim_I = \{V_1, \dots, V_k\}$ (resp. $E(G)/\sim_I = \{E_1, \dots, E_k\}$) be its equivalence classes and let $v_i \in V_i$ (resp. $e_i \in E_i$) for $i \in [k] = \{1, \dots, k\}$. Then (1) can be rewritten as

$$I(G) = \sum_{i=1}^k |V_i| f(v_i), \quad (3)$$

while (2) reduces to

$$I(G) = \sum_{i=1}^k |E_i| f(e_i). \quad (4)$$

The value k is called the *I-complexity* of G and denoted $C_I(G)$. This concept was introduced in [3] and studied on the connective eccentricity index; see [11, 29] for more information on the latter index. Earlier, the complexity with respect to the Wiener index was investigated in [2] under the name Wiener dimension.

The paper is organized as follows. In the next section additional concepts needed are introduced. In the central part of the paper, Section 3, the Sz-complexity of graphs is compared to the numbers of their edge orbits O_e and the number of their vertex orbits O_v . It is observed that for any graph G , $C_{Sz}(G) \leq O_e(G)$, and demonstrated that for any integer $m \geq 1$ there exists a vertex-transitive graph G_m with $C_{Sz}(G_m) = O_e(G_m) = m$. Moreover, for any $1 \leq k \leq m+1$ there exists a graph $G_{m,k}$ with $C_{Sz}(G_{m,k}) = O_e(G_{m,k}) =$

m and $C_W(G_{m,k}) = O_v(G_{m,k}) = k$. In Section 4 the Sz-complexity is determined for a family of (5,0)-nanotubical fullerenes. As a consequence the Szeged index of these fullerenes is determined. In the final section it is proved that if G is a connected graph of order at least 4, then $\text{Sz}(G) \geq \text{Ecc}(G)$, where equality holds if and only if $G = P_4$.

2 Preliminaries

All graphs considered in this paper are connected. The *degree* of a vertex u of a graph G is denoted with $\deg_G(u)$. The *distance* between vertices u and v of a graph G is denoted by $d_G(u, v)$. The *distance* $d_G(v)$ of vertex v is defined as $d_G(v) = \sum_{u \in V(G)} d_G(v, u)$. The *eccentricity* $\text{ecc}_G(v)$ of v is the largest distance between v and the vertices of G . Whenever G is clear from the context, we may omit the index G in the above notation. The maximum and the minimum eccentricity among all vertices of G are the *diameter* $\text{diam}(G)$ and the *radius* $\text{rad}(G)$, respectively.

The *Wiener index* of graph G is the sum of distances between all pairs of vertices of G , that is,

$$W(G) = \frac{1}{2} \sum_{v \in V(G)} d(v).$$

Let $e = uv$ be an edge of graph G . The number of vertices of G lying closer to u than to v is denoted by $n_u(e)$. Analogously, $n_v(e)$ is the number of vertices of G lying closer to v than to u . The *Szeged index* [13] of G is defined with

$$\text{Sz}(G) = \sum_{e=uv \in E(G)} n_u(e)n_v(e).$$

The *total eccentricity* of G is defined as

$$\text{Ecc}(G) = \sum_{v \in V(G)} \text{ecc}(v).$$

Let $\text{Aut}(G)$ denote the automorphism group of G . A graph G is *vertex-transitive* if to any vertices u and v of G there exists $\alpha \in \text{Aut}(G)$ such that $\alpha(u) = v$. Let $O_v(G)$ and $O_e(G)$ be the number of vertex orbits and edge orbits of G under the action of $\text{Aut}(G)$, respectively. A function $f : V(G) \rightarrow \mathbb{R}$ (resp. $f : E(G) \rightarrow \mathbb{R}$) is a *graph function* if it is invariant under automorphisms of G ; that is, if $\alpha \in \text{Aut}(G)$ and u and u' belong to the same vertex orbit (resp. e and e' belong to the same edge orbit), then $f(u) = f(u')$ (resp. $f(e) = f(e')$).

We will use the following result that goes back to [10].

Proposition 2.1 *If $e = uv$ is an edge of a connected graph G , then $d_G(u) - d_G(v) = n_v(e) - n_u(e)$.*

3 Sz-complexity versus number of edge orbits

Suppose that a topological index I is of the form (1) or (2), where f is a graph function. Then by definition,

$$C_I(G) \leq O_v(G) \quad (\text{resp. } C_I(G) \leq O_e(G)). \quad (5)$$

We note in passing that if $C_I(G) \leq O_v(G)$, then $C_I(G) \leq O_e(G) + 1$. This follows from a result of Buset [7] asserting that if G a (connected) graph, then $O_v(G) \leq O_e(G) + 1$.

Theorem 3.1 *If G is a graph, then $C_{\text{Sz}}(G) \leq O_e(G)$. Moreover, for any integer $m \geq 1$ there exists a vertex-transitive graph G_m with $C_{\text{Sz}}(G_m) = O_e(G_m) = m$.*

Proof. For the first assertion, in view of (5) it suffices to prove that the function $f(e) = n_u(e)n_v(e)$, where $e = uv \in E(G)$, is a graph function. Hence let $e = uv$ and $e' = xy$ be edges from the same edge orbit, and let $\alpha \in \text{Aut}(G)$ such that $\alpha(u) = x$ and $\alpha(v) = y$. Let $\Gamma_k(u) = \{w \in V(G) \mid d(u, w) = k\}$, $0 \leq k \leq \text{ecc}(u)$. We claim that $n_u(e) = n_x(e')$ and $n_v(e) = n_y(e')$. For this sake observe first that $n_u(uv) = \sum_{k=0}^{\text{ecc}(u)} |\Gamma_k(u) \cap \Gamma_{k+1}(v)|$. Furthermore,

$$w \in \Gamma_k(u) \cap \Gamma_{k+1}(v) \Leftrightarrow \alpha(w) \in \Gamma_k(\alpha(u)) \cap \Gamma_{k+1}(\alpha(v)) = \Gamma_k(x) \cap \Gamma_{k+1}(y).$$

Therefore

$$n_u(uv) = \sum_{k=0}^{\text{ecc}(u)} |\Gamma_k(u) \cap \Gamma_{k+1}(v)| = \sum_{k=0}^{\text{ecc}(x)} |\Gamma_k(x) \cap \Gamma_{k+1}(y)| = n_x(xy).$$

This proves the first assertion of the theorem.

Let $m \geq 1$ and set $n = 3m + 1$. Define the graph G_m on the vertex set $[n]_0 = \{0, 1, \dots, n-1\}$, where the vertex i is adjacent to vertices $i \pm 1, \dots, i \pm m \pmod{n}$. Clearly, G_m is vertex-transitive. (Alternatively, G_m belong to the family of circulant graphs which are well-known to be vertex-transitive.) Consider now the edge ij , where $j = i \pm k$, $1 \leq k \leq m$. Then ij lies in precisely $m - k + 1$ complete subgraphs K_{m+1} . It follows that G_m contains at least m edge orbits. On the other hand, any two edges that differ by the same integer, are in the same edge orbit. We conclude that $O_e(G_m) = m$. Finally, any

pair of vertices has a common adjacent vertex, hence $\text{diam}(G_m) = 2$. Moreover, since G_m is $(2m)$ -regular, vertices i and $j = i \pm k$, $1 \leq k \leq m$, have exactly $2m - k - 1$ common adjacent vertices. Consequently $n_i(ij) = n_j(ij) = k + 1$. Therefore, $C_{\text{Sz}}(G_m) = m$. \square

In view of (5) the reader might wonder why the first assertion of Theorem 3.1 requires a proof. To see that the assertion need not be true in general, consider the following example. Let G be a graph with the vertex set $[n]_0$, and define the invariant $\text{Sz}'(G) = \sum_{e=ij \in E(G)} n_i(e) - n_j(e)$. Then in general $C_{\text{Sz}'}(G) \leq O_e(G)$ does not hold. For a small example consider the path P_3 of order 3. Clearly, $O_e(P_3) = 1$, but $C_{\text{Sz}'}(P_3) = 2$.

In Theorem 3.1 we have seen that there exist graphs with a single vertex orbit and with an arbitrary large Sz-complexity. On the other hand, we also have:

Proposition 3.2 *There exists an infinite family of non edge-transitive graphs with Sz-complexity equal to 1.*

Proof. Let W_n , $n \geq 3$, be the n -wheel, that is, the graph obtained from the n -cycle C_n and an extra vertex joined to all the vertices of the cycle. The cogwheel M_n is then obtained from W_n by subdividing each edge of C_n by one vertex. Clearly, M_n is not edge-transitive. On the other hand it is straightforward to infer that for any edge $e = uv \in E(M_n)$ we have $\{n_u(e), n_v(e)\} = \{3, 2n - 2\}$, so that $C_{\text{Sz}}(M_n) = 1$. \square

It is straightforward to see that the cogwheel M_n has two edge orbits. Hence an interesting question appears whether there exist (infinite families of) graphs with Sz-complexity equal to 1 and with an arbitrary number of edge orbits.

By the above-mentioned Buset's result [7] we have $O_v(G) \leq O_e(G) + 1$. We next show that comparing the Sz-complexity with the W-complexity anything else can happen. More precisely:

Theorem 3.3 *If $m \geq 1$ and $1 \leq k \leq m + 1$, then there exists a graph $G_{m,k}$ with $C_{\text{Sz}}(G_{m,k}) = O_e(G_{m,k}) = m$ and $C_W(G_{m,k}) = O_v(G_{m,k}) = k$.*

Proof. Let $m \geq 1$ and set $G_{m,m+1} = P_{2m+1}$. Then it can be routinely checked that $C_{\text{Sz}}(G_{m,m+1}) = O_e(G_{m,m+1}) = m$ and $C_W(G_{m,m+1}) = O_v(G_{m,m+1}) = m + 1$.

Suppose in the rest that $m \geq 1$ and $1 \leq k \leq m$. Let G_m be the graph of order $3m + 1$ as constructed in the proof of Theorem 3.1, where $V(G_m) = [3m + 1]_0$. Let $G_{m,k}$ be the graph obtained from a disjoint union of G_{m-k+1} and $m - k + 1$ copies of the path P_k , by

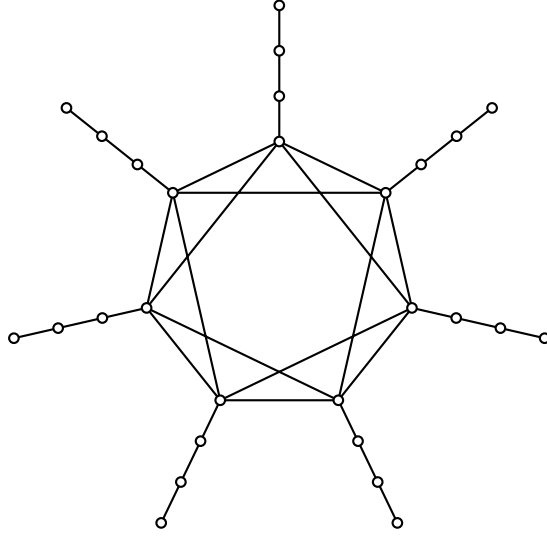


Figure 1: The graph $G_{5,4}$

identifying each of the vertices of G_{m-k+1} with an end-vertex of a respective copy of P_k . The construction is illustrated in Fig. 1 with the graph $G_{5,4}$. Note also that $G_{m,1} = G_m$.

As already inferred in the proof of Theorem 3.1, $O_e(G_{m-k+1}) = m - k + 1$. This in turn implies that $O_e(G_{m,k}) = (m - k + 1) + (k - 1) = m$. Consider now the edges $0j$, $j \in [m - k + 1]$, of G_{m-k+1} (considered as a subgraph of $G_{m,k}$), and observe that $a_j = n_0(0j) = n_j(0j) = (j + 1)k$. Furthermore, for the $k - 1$ edges e_i of an arbitrary fixed attached P_k , we easily infer that their contributions to the Szeged index are $b_i = i(3k(m - k + 1) + k - i)$, $i \in [k - 1]$, because $|V(G_{m,k})| = 3k(m - k + 1) + k$. Since for any $i \in [k - 1]$ and any $j \in [m - k + 1]$ we have $i(3k(m - k + 1) + k - i) > (j + 1)k$, there exist $(m - k + 1) + (k - 1) = m$ different contributions to $\text{Sz}(G_{m,k})$. Hence in view of the second assertion of (5) and the above fact that $O_e(G_{m,k}) = m$ we conclude that $C_{\text{Sz}}(G_{m,k}) = m$.

Since G_{m-k+1} is vertex-transitive, it follows directly that $O_v(G_{m,k}) = k$. Moreover, by symmetry, all the vertices of G_{m-k+1} (considered as vertices of $G_{m,k}$) have the same distance in $G_{m,k}$. Consider now the vertices of an arbitrary fixed P_k subgraph of $G_{m,k}$. Then by iterative applications of Proposition 2.1 we get that all these k vertices have different distances. Hence by the first assertion of (5) we conclude that $C_W(G_{m,k}) = k$. \square

Considering the graphs from the proof of Theorem 3.3 and noting that $C_{\text{Ecc}}(P_{2m+1}) = m + 1$ for $m \geq 1$ and that $C_{\text{Ecc}}(G_{m,k}) = k$ for $m \geq 1$ and $1 \leq k \leq m$, we get in passing

the following result.

Corollary 3.4 *If $m \geq 1$ and $1 \leq k \leq m + 1$, then there exists a graph $G_{m,k}$ with $C_{\text{Sz}}(G_{m,k}) = O_e(G_{m,k}) = m$ and $C_{\text{Ecc}}(G_{m,k}) = O_v(G_{m,k}) = k$.*

4 Sz-complexity of the fullerenes C_{10n}

In this section we compute the Sz-complexity of a family of fullerene graphs. This yields another infinite family of (chemical) graphs for which the Sz-complexity coincides with the number of edge orbits.

A fullerene graph is a 3-connected, 3-regular plane graph with only pentagonal and hexagonal faces. They have exactly twelve pentagonal faces. Here we consider the family of fullerenes C_{10n} , $n \geq 2$, known as (5,0)-nanotubical fullerenes. (For distance properties of C_{10n} see [2, 4].) The fullerene C_{10n} contains $10n$ vertices which are grouped into $n + 1$ layers L_0, L_1, \dots, L_n , where the layers L_0 and L_n contain 5 vertices, while each of the other layers contains 10 vertices. In Fig. 2 the case $n = 5$ is drawn, that is, C_{50} , from which the general edge structure of these graphs should be clear.

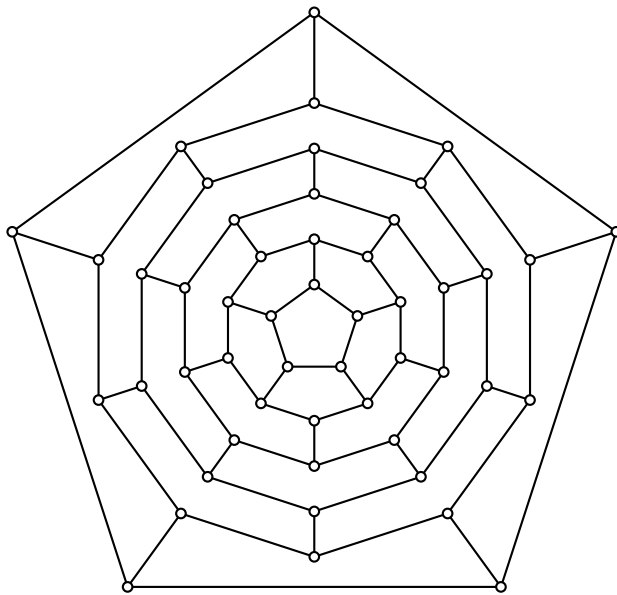


Figure 2: The C_{50} fullerene

The main result of this section reads as follows.

Theorem 4.1 *If $n \geq 3$, then $C_{\text{Sz}}(C_{10n}) = n + 1 = O_e(C_{10n})$.*

Proof. Let L_0, L_1, \dots, L_n be the layers of vertices of C_{10n} , and let S_i be the set of edges connecting a vertex of L_{i-1} to a vertex of L_i . It is not difficult to observe that for $0 \leq i \leq \lfloor \frac{n+1}{2} \rfloor$, the edges of L_i and L_{n-i} are in the same orbit and that for $1 \leq j \leq \lfloor \frac{n}{2} \rfloor$, the edges of S_j and edges of S_{n-j} are in the same edge orbit. Hence, using Theorem 3.1, $C_{S_z}(C_{10n}) \leq O_e(C_{10n}) = n + 1$.

We checked by computer that $C_{S_z}(C_{10n}) = n + 1$ holds for $3 \leq n \leq 9$. In the rest we prove by induction that the same holds for $n \geq 9$. To simplify the notation, set $N(e) = n_u(e)n_v(e)$ for an edge $e = uv$. For $n = 9, 10$, let $e_i \in L_i$, $0 \leq i \leq \lfloor \frac{n}{2} \rfloor$ and $f_j \in S_j$ for $1 \leq j \leq \lfloor \frac{n+1}{2} \rfloor$. With the help of computer again we have obtained the corresponding values for C_{90} and C_{100} as given in Table 1.

i	$N(e_i)$	$N(f_i)$
0	12×12	-
1	18×70	9×69
2	24×64	15×75
3	32×57	25×65
4	40×49	35×55
5	-	45×45

i	$N(e_i)$	$N(f_i)$
0	12×12	-
1	18×80	9×79
2	24×74	15×85
3	32×67	25×75
4	40×59	35×65
5	50×50	45×55

Table 1: Values $N(e)$ for the edges of C_{90} (left) and of C_{100} (right)

Let $e = uv$ be an arbitrary edge of C_{10n} . We distinguish three typical cases with respect to the position of uv .

Suppose first that uv lies within L_0 or L_{n+1} . Then for $n = 3$ one can check that $n_u(e) = 10$, while if $n \geq 4$, then $n_u(e) = 12$. The latter fact is illustrated in Fig. 3, where the vertices closer to u than to v are colored blue and the vertices closer to v than to u red.

Suppose next that $e = uv \in S_i$ for $1 \leq i \leq \lfloor \frac{n}{2} \rfloor$. Since we will consider the edge e in fullerenes C_{10n} and in $C_{10(n+1)}$, hence we specify the notation $n_u(e)$ to $n_u^{(n)}(e)$, meaning that we consider e in C_{10n} . Now we have $N_u^{(n+1)}(e) = N_u^{(n)}(e)$ and $n_v^{(n+1)}(e) = n_v^{(n)}(e) + 10$ (or vice versa). In addition, when n is odd and $uv \in S_{\lfloor \frac{n+1}{2} \rfloor}$, then $n_u^{(n)}(e) = N_v^{(n)}(e) = 5n$.

Assume finally that $uv \in L_i$, where $1 \leq i \leq \lfloor \frac{n-1}{2} \rfloor$, the vertex u is adjacent to some vertex of L_{i-1} , and the vertex v is adjacent to some vertex of L_{i+1} . Now $n_u^{(n+1)}(e) = n_v^{(n)}(e)$ and $n_v^{(n+1)}(e) = n_v^{(n)}(e) + 10$. If n is even, then for the edge $uv \in L_{\frac{n}{2}}$ we have $n_u^{(n)}(e) = N_v^{(n)}(e) = 5n$.

From the above consideration we conclude that $C_{S_z}(C_{10(n+1)}) = C_{S_z}(C_{10n}) + 1 = n + 2$ which completes the inductive argument. \square

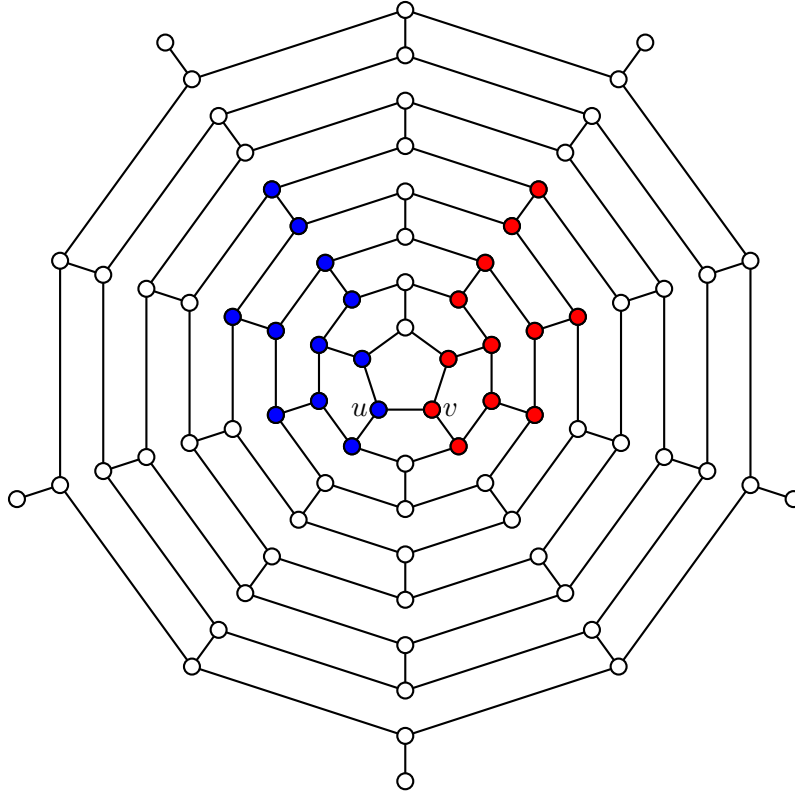


Figure 3: If $e = uv$ lies in L_0 , then $n_u(e) = n_v(e) = 12$

As a consequence of Theorem 4.1, together with a help of computer, we can also determine the Szeged index of the fullerenes C_{10n} .

Corollary 4.2 $Sz(C_{30}) = 6655$, $Sz(C_{40}) = 16830$, $Sz(C_{50}) = 33545$, $Sz(C_{60}) = 58900$, $Sz(C_{70}) = 93535$, $Sz(C_{80}) = 138810$. Moreover, if $n \geq 9$, then

$$Sz(C_{10n}) = 250n^3 + 3075n - 13800.$$

5 Szeged index versus total eccentricity

The relation between the Szeged index and the Wiener index has already been well investigated. In [21] it was first proved that $Sz(G) \geq W(G)$ holds for any connected graph. Moreover, the equality holds if and only if G is a block graph [9, 26]. The inequality was in [19] extended by proving that $Sz(G, w) \geq W(G, w)$ holds for any connected network. In addition, in [20, 23, 24, 30] bounds on $Sz(G) - W(G)$ and graphs achieving a fixed value

of the difference were investigated. In this section we compare the Szeged index with the total eccentricity (cf. [27]) and prove the following result.

Theorem 5.1 *If G is a connected graph of order at least 4, then $\text{Sz}(G) \geq \text{Ecc}(G)$. Moreover, equality holds if and only if $G = P_4$.*

Proof. It is straightforward to verify that $\text{Sz}(G) > \text{Ecc}(G)$ holds if $G = C_n$, $n \geq 4$ or if $G = P_n$, $n \geq 5$. Hence assume in the rest that G is a connected graph of order at least 4 that is neither a path nor a cycle. In particular, G contains a vertex of degree at least 3.

Let $v \in V(G)$ and let v' be a vertex with $d(v, v') = \text{ecc}(v)$. Considering a shortest v, v' -path we infer that $d(v) \geq 1 + \dots + \text{ecc}(v)$. Moreover, since G is not a path, it contains at least one vertex that does not lie on P_v and consequently

$$d(v) \geq (1 + \dots + \text{ecc}(v)) + 1 = \frac{\text{ecc}(v)(\text{ecc}(v) + 1)}{2} + 1 \geq 2\text{ecc}(v),$$

where the latter inequality reduces to $\text{ecc}(v)^2 + 2 \geq 3\text{ecc}(v)$ which can be easily verified to hold true.

We have thus shown that $d(v) \geq 2\text{ecc}(v)$ holds for any vertex v of G . Moreover, since G contains at least one vertex, say w , of degree at least 3, by the above argument, but adding 2 instead of 1, we have $d(w) > 2\text{ecc}(w)$. Therefore

$$\sum_{v \in V(G)} d(v) > \sum_{v \in V(G)} 2\text{ecc}(v) = 2\text{Ecc}(G).$$

This implies that $W(G) > \text{Ecc}(G)$. Since, as mentioned before the theorem, $\text{Sz}(G) \geq W(G)$ holds for any connected graph G , we conclude that $\text{Sz}(G) > \text{Ecc}(G)$. \square

Theorem 5.1, together by considering the graphs K_2 , K_3 , and P_3 , yields:

Corollary 5.2 *If G is a connected graph with at least one edge, then $\text{Sz}(G) = \text{Ecc}(G)$ if and only if $G \in \{K_3, P_4\}$.*

To conclude the paper we add that a comparison between the Szeged index and the eccentric connectivity index was done in [8].

Acknowledgements

The second author acknowledges the project (Exploration of the intrinsic structure of Tower graphs, J1-7110) was financially supported by the Slovenian Research Agency. The author also acknowledge the financial support from the Slovenian Research Agency (research core funding No. P1-0297).

References

- [1] Y. Alizadeh, Szeged dimension and PI_v dimension of composite graphs, *Iranian J. Math. Sci. Inform.*, to appear.
- [2] Y. Alizadeh, V. Andova, S. Klavžar, R. Škrekovski, Wiener dimension: fundamental properties and (5,0)-nanotubical fullerenes, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 279–294.
- [3] Y. Alizadeh, S. Klavžar, Complexity of topological indices: The case of connective eccentric index, *MATCH Commun. Math. Comput. Chem.* **76** (2016) 659–667.
- [4] V. Andova, T. Došlić, M. Krnc, B. Lužar, R. Škrekovski, On the diameter and some related invariants of fullerene graphs, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 109–130.
- [5] M. Arockiaraj, J. Clement, K. Balasubramanian, Analytical expressions for topological properties of polycyclic benzenoid networks, *J. Chemometrics* **30** (2016) 682–697.
- [6] M. Arockiaraj, J. Clement, A.J. Shalini, Variants of the Szeged index in certain chemical nanosheets, *Canad. J. Chem.* **94** (2016) 608–619.
- [7] D. Buset, Orbits on vertices and edges of finite graphs, *Discrete Math.* **57** (1985) 297–299.
- [8] K.Ch. Das, M.J. Nadjafi-Arani, Comparison between the Szeged index and the eccentric connectivity index, *Discrete Appl. Math.* **186** (2015) 74–86.
- [9] A.A. Dobrynin, I. Gutman, Solving a problem connected with distances in graphs, *Graph Theory Notes New York* **28** (1995) 21–23.
- [10] R.C. Entringer, D.E. Jackson, D.A. Snyder, Distance in graphs, *Czechoslovak Math. J.* **26** (1976) 283–296.
- [11] S. Gupta, M. Singh, A.K. Madan, Connective eccentricity index: a novel topological descriptor for predicting biological activity, *J. Mol. Graph. Model.* **18** (2000) 18–25.
- [12] M. Goubko, O. Miloserdov: Simple alcohols with the lowest normal boiling point using topological indices *MATCH Commun. Math. Comput. Chem.* **75** (2016) 29–56.
- [13] I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, *Graph Theory Notes N. Y.* **27** (1994) 9–15.
- [14] I. Gutman, B. Furtula (Eds.), *Novel Molecular Structure Descriptors—Theory and Applications I*, Univ. Kragujevac, Kragujevac, 2010.
- [15] I. Gutman, B. Furtula (Eds.), *Novel Molecular Structure Descriptors—Theory and Applications II*, Univ. Kragujevac, Kragujevac, 2010.

- [16] I. Gutman, K. Xu, M. Liu, A congruence relation for Wiener and Szeged indices, *Filomat* **29** (2015) 1081–1083.
- [17] M. Imran, A.Q Baig, H. Ali, On molecular topological properties of hex-derived networks, *J. Chemometrics* **30** (2016) 121–129.
- [18] P.V. Khadikar, S. Karmarkar, V.K. Agrawal, J. Singh, A. Shrivastava, I. Lukovits, M.V. Diudea, Szeged index - applications for drug modeling, *Lett. Drug Des. Discov.* **2** (2005) 606–624
- [19] S. Klavžar, M.J. Nadjafi-Arani, Wiener index versus Szeged index in networks, *Discrete Appl. Math.* **161** (2013) 1150–1153.
- [20] S. Klavžar, M.J. Nadjafi-Arani, Improved bounds on the difference between the Szeged index and the Wiener index of graphs, *European J. Combin.* **39** (2014) 148–156.
- [21] S. Klavzar, A. Rajapakse, I. Gutman, The Szeged and the Wiener index of graphs, *Appl. Math. Lett.* **9** (1996) 45–49.
- [22] S. Li, H. Zhang, Proofs of three conjectures on the quotients of the (revised) Szeged index and the Wiener index and beyond, *Discrete Math.* **340** (2017) 311–324.
- [23] M. J. Nadjafi-Arani, H. Khodashenas, A. R. Ashrafi, On the differences between Szeged and Wiener indices of graphs, *Discrete Math.* **311** (2011) 2233–2237.
- [24] M. J. Nadjafi-Arani, H. Khodashenas, A. R. Ashrafi, Graphs whose Szeged and Wiener numbers differ by 4 and 5, *Math. Comput. Modelling* **55** (2012) 1644–1648.
- [25] F. Shafiei, M. Pashm Froush, F. Dialamehpour, QSPR study on benzene derivatives to some physicochemical properties by using topological indices, *Iranian J. Math. Chem.* **7** (2016) 93–110.
- [26] S. Simić, I. Gutman, V. Baltić, Some graphs with extremal Szeged index, *Math. Slovaca* **50** (2000) 1–15.
- [27] H. Smith, L. Székely, H. Wang, Eccentricity sums in trees, *Discrete Appl. Math.* **207** (2016) 120–131.
- [28] R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatic*, Wiley-VCH, Weinheim, 2009.
- [29] K. Xu, K.Ch. Das, H. Liu, Some extremal results on the connective eccentricity index of graphs, *J. Math. Anal. Appl.* **433** (2016) 803–817.
- [30] H. Zhang, S. Li, L. Zhao, On the further relation between the (revised) Szeged index and the Wiener index of graphs, *Discrete Appl. Math.* **206** (2016) 152–164.