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Note on the graphs with the greatest edge-Szeged index

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Abstract

Recently, it was conjectured that the complete graph K_n has the greatest edge-Szeged index among all simple graphs with n vertices. In this paper it is shown that this conjecture is not true. Moreover, the asymptotic behavior of edge-Szeged index is analyzed. Also, the maximum value of edge-Szeged index for graphs with m edges is found and the extremal graphs are identified.

1. Introduction

The Wiener index [1] is one of the most famous topological indices [2, 3] and it is defined by

$$W(G) = \sum_{u,v \in V(G)} d_G(u,v), \tag{1}$$

where $d_G(u,v)$ is distance of vertices u and v, $V(G)$ is the set of vertices of the graph G and the summation runs through all pairs of vertices. It has been shown that Wiener index for acyclic connected graph G is equal to

$$W(G) = \sum_{uv \in E(G)} n_u(uv \mid G) \cdot n_v(uv \mid G), \tag{2}$$

where $n_u(uv \mid G)$ is the number of vertices (in graph G) closer to vertex u then to vertex v, $n_v(uv \mid G)$ is the number of vertices closer to vertex v then to vertex u, and the summation runs through the set of edges $E(G)$ of G. These two formulas have been inspiration for definition of many similar topological indices. Formula (1) has been extended [4] to

$$W_{\lambda}(G)=\sum_{u,v\in V(G)} d_G(u,v)^{\lambda}$$

and formula (2) was extended (for acyclic connected graphs) to [5,6]

$$^{m}W_{\lambda}(G)=\sum_{uv\in E(G)}\left[n_u(uv\,|\,G)\cdot n_v(uv\,|\,G)\right]^{\lambda}$$

$$W_{\min,\lambda}(G)=\sum_{uv\in E(G)}\left(n(G)^{\lambda}\cdot\min\left\{n_u(uv\,|\,G),n_u(uv\,|\,G)\right\}^{\lambda}-\min\left\{n_u(uv\,|\,G),n_u(uv\,|\,G)\right\}^{2\lambda}\right),$$

Where $n(G)$ is number of vertices in G. Properties of these indices have been analyzed in [7-9]

Extending formula (2) to all graphs Szeged index [10] has been obtained:

$$Sz(G)=\sum_{uv\in E(G)} n_u(uv\,|\,G)\cdot n_v(uv\,|\,G)$$

Obviously, Wiener index and Szeged index coincide for acyclic graphs, but they differ for cyclic graphs. Properties of the Szeged index have been extensively studied (see paper [11] and references within).

Recently, a modification of this index has been proposed. Namely, edge-version of Szeged index [12] was proposed by:

$$Sz_e(G)=\sum_{uv\in E(G)} m_u(uv\,|\,G)\cdot m_v(uv\,|\,G),$$

where $m_u(uv\,|\,G)$ is the number of edges (in graph G) closer to vertex u then to vertex v and $m_v(uv\,|\,G)$ is the number of edges closer to vertex v then to vertex u

In the same paper several properties of this index have been analyzed and the following conjecture has been proposed:

Conjecture 1. The complete graph K_n has the greatest edge-Szeged index among all simple graphs with n vertices.

Also, it has been shown that $Sz_e(K_n)=\frac{1}{2}n(n-1)^3$.

2. Main results

In this paper Conjecture 1 is refuted, moreover it will be proved that:

Theorem 2. $\lim_{n\to\infty} \log_n \max\left\{Sz_e(G) : G \text{ is a simple graph with } n \text{ vertices}\right\} = 6$.

Note that $\lim_{n\to\infty} \log_n Sz_e(K_n) = 4$, hence for sufficiently large n, Conjecture 1 is not true. It will be also proved that:

Theorem 3. Let G be a graph (possibly with multiple bonds) with $m \geq 5$ edges. Then,

$$Sz_e(G) \leq \begin{cases} m\cdot(m-1)^2/4, & m \text{ is odd;} \\ (m+2)\cdot(m-2)^2/4, & m \text{ is even.} \end{cases}$$

Both inequalities are tight. In the even case, the equality is obtained only for the cycle with m vertices and in odd case the equality is obtained only for the cycle with $m-1$ vertices with one double bond.

The examples of the extremal graphs with $m=6$ and $m=7$ are given on the following figure:

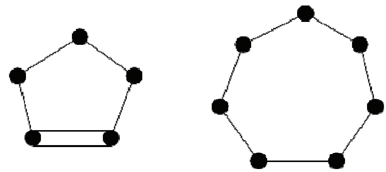

Figure 1. Extremal grapsh for $m=6$ and $m=7$.

These graphs will be denoted by C_{m-1}^d and C_m.

Finally, as an open problem, the following conjecture is proposed:

Conjecture 4. $\lim_{n\to\infty} \frac{\max\left\{Sz_e(G) : G \text{ is a simple graph with } n \text{ vertices}\right\}}{n^6} = \frac{1}{15552}$.

3. Proof of the Theorem 2

Simple graph with n vertices has at most $\binom{n}{2}$ edges, hence contribution of each edge can be at most $\left\lfloor \binom{n}{2} - 1 \right\rfloor \cdot \left\lceil \binom{n}{2} - 1 \right\rceil$, where $\lfloor x \rfloor$ is the greatest integer smaller or equal to x; and $\lceil x \rceil$ is the smallest integer greater or equal to x. Therefore, edge-Szeged index of simple graph with n vertices is at most $\binom{n}{2} \cdot \left\lfloor \binom{n}{2} - 1 \right\rfloor \cdot \left\lceil \binom{n}{2} - 1 \right\rceil$. Hence,

$$\lim_{n\to\infty} \log_n \max\left\{Sz_e(G) : G \text{ is a simple graph with } n \text{ vertices}\right\} \leq$$
$$\leq \lim_{n\to\infty} \log_n \left\{\binom{n}{2}\cdot\left\lfloor\binom{n}{2}-1\right\rfloor\cdot\left\lceil\binom{n}{2}-1\right\rceil\right\} = 6.$$

On the other hand, let G_n, $n \geq 9$ be graph given by:

$$V(G_n) = \left\{v_{i,j} : (i,j) \in S\right\},$$

where

$$S = \left\{(i,j) : i \in \{0,1,3,4,6\} 1 \leq j \leq \left\lfloor \frac{n-3}{6} \right\rfloor\right\} \cup \left\{(i,1) : i \in 2,5,8\right\} \cup \left\{(7,j) : 1 \leq j \leq n-3-5\cdot\left\lfloor \frac{n-3}{6} \right\rfloor\right\};$$

and

$$E(G_n) = \left\{v_{i,j}v_{k,l} : i-k \equiv 1(\text{mod}\, 9)\right\}.$$

In order to illustrate this definition, we present graph G_{16} on the following figure:

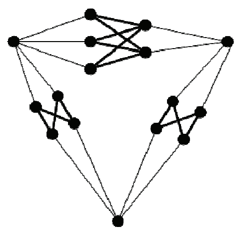

Figure 2. Graph G_{16}

Note that each bold edge contributes to the sum more then $\left\lfloor \frac{n-3}{6} \right\rfloor^2 \cdot \left\lfloor \frac{n-3}{6} \right\rfloor^2$. Hence,

$$Sz_e(G_n) > 3\cdot\left\lfloor \frac{n-3}{6} \right\rfloor^6.$$

Therefore,

$$\lim_{n\to\infty} \log_n \max\left\{Sz_e(G) : G \text{ is a simple graph with } n \text{ vertices}\right\} \geq$$
$$\geq \lim_{n\to\infty} \log_n \left\{3\cdot\left\lfloor \frac{n-3}{6} \right\rfloor^6\right\} = 6.$$

Hence, both inequalities are proved and therefore:

$$\lim_{n\to\infty} \log_n \max\left\{Sz_e(G): G \text{ is a simple graph with } n \text{ vertices}\right\} = 6.$$

Remark Tedious calculation shows that for these graphs, it holds:

$$\lim_{n\to\infty} \frac{Sz_e(G_n)}{n^6} = \frac{1}{15552},$$

which inspired Conjecture 4.

4. Proof of the Theorem 3

Distinguish two cases:

CASE 1: m is odd.

Each edge can contribute at most $\left(\frac{m-1}{2}\right)^2$. Hence,

$$Sz_e(G) \le m \cdot \left(\frac{m-1}{2}\right)^2 = m \cdot (m-1)^2 / 4.$$

It can be easily checked that equality holds for the even cycle. Let us prove that equality can not hold for any other graph. Suppose to the contrary that equality holds for the graph $H \ne C_m$. Then, each edge in H contributes $\left(\frac{m-1}{2}\right)^2$. Therefore, H has no loops, nor double bonds (i.e. H is simple). Also, H is connected and has no pendant edges. Therefore H has at least one cycle that does not pass through all vertices. Let C_H be the smallest cycle in H. Since $H \ne C_m$, there is an edge connecting vertex in $V(C_H)$ and vertex in $V(H \setminus C_H)$. Denote this vertex by $v_0 w$ and vertices in cycle C_H (in order of their appearance) by $v_0, v_1 ..., v_{k-1}$. Distinguish two subcases:

SUBCASE 1.1: k is even.

Note that $d(v_0, v_{k/2}) \ge \frac{k}{2}$ and that $d(v_0, v_{k/2+1}) \ge \frac{k}{2} - 1$, because otherwise there would be a smaller cycle in H. Hence $d(v_0, v_{k/2}) = \frac{k}{2}$ and $d(v_0, v_{k/2+1}) = \frac{k}{2} - 1$. Analogously, it can be shown that $d(v_1, v_{k/2}) = \frac{k}{2} - 1$ and $d(v_1, v_{k/2+1}) = \frac{k}{2}$. Hence, edge $v_{k/2} v_{k/2+1}$ is on the same distance from v_0 and v_1 which is in contradiction with the fact that edge $v_0 v_1$ contributes $\left(\frac{m-1}{2}\right)^2$.

SUBCASE 1.2: k is odd.

Note that $d\left(v_0, v_{(k-1)/2}\right), d\left(v_0, v_{(k+1)/2}\right) \geq \frac{k-1}{2}$, because otherwise there would be a smaller cycle in H. Hence, $d\left(v_0, v_{(k-1)/2}\right), d\left(v_0, v_{(k+1)/2}\right) = \frac{k-1}{2}$. Similarly, it can be shown that $d\left(w, v_{(k-1)/2}\right), d\left(w, v_{(k+1)/2}\right) \geq \frac{k-1}{2}$. Therefore edge $v_0 w$ is on the same distance from v_0 and v_1 which is in contradiction with the fact that edge $v_0 v_1$ contributes $\left(\frac{m-1}{2}\right)^2$.

CASE 2: m is even.

It can be easily seen that the equality holds for the cycle with $m-1$ vertices and one double bond. It remains to show that for all other graphs edge-Szeged index is smaller then $\left(m^2-2\right)\cdot\left(m-2\right)/4$. Suppose to the contrary that there is a graph $H \neq C_{m-1}^d$ such that

$$Sz_e\left(H\right) \geq \left(m-2\right)^2 \cdot \left(m+2\right)/4 .$$

Since, each edge can contribute at most $m\left(m-2\right)/4$, it follows that each edge in H contributes at least

$$\left(m-2\right)^2 \cdot \left(m+2\right)/4 - \left(m-1\right)m\left(m-2\right)/4 = \left(m-2\right)\left(m-4\right)/4 .$$

This implies that h has no loops nor pendant vertices. Distinguish two subcases:

SUBCASE 2.1: H has at least one multiple bond.

Note that each of the edges in double bond contributes at most $\left(m-2\right)^2/4$. Since

$$\left(m-2\right)\cdot\frac{m}{2}\cdot\frac{m-2}{2} + 2\cdot\left(\frac{m-2}{2}\right)^2 = \left(m+2\right)\cdot\left(m-2\right)^2/4$$

Hence, it follows that there are at most two edges engaged in double bonds. Therefore, there is only one double bond in the graph and all edges have maximal possible contributions, i.e. single bonds contribute $\frac{m\left(m-2\right)}{4}$ and two edges in double bonds contribute $\frac{\left(m-2\right)^2}{4}$ each. Contradiction in this subcase can be obtianed similarly as in the Case 1 by observing the shortest cycle (where double bond is not counted as a cycle) and showing that at least one edge will not contribute this maximal value.

SUBCASE 2.2: H is a simple graph

Let C_H be the shortest cycle. It can be easily seen that C_H does not pass thorugh all vertices. As in Case 1, there is an edge connecting vertex in $V(C_H)$ and vertex in $V(H \setminus C_H)$. Denote $v_0,...,v_{k-1}$ and w as in the Case 1. Distinguish two subcases:

SUBCASE 2.2.1: k is even.

Similarly, as in the Subcase 1.1, it can be shown that edge $v_{i+k/2,i+k/2+1}$ is on the same distance from vertices v_i and v_{i+1} (where addition is taken modulo k). Therefore, each edge in the cycle contributes at most $\left(\frac{k-2}{2}\right)^2$, but then

$$Sz_e(H)=(m-k)\cdot\frac{m(m-2)}{4}+k\frac{(m-2)^2}{4}=$$
$$(m+2)\cdot(m-2)^2/4-(k-2)\left(\frac{m(m-2)}{4}-\frac{(m-2)^2}{4}\right)<$$
$$<(m+2)\cdot(m-2)^2/4,$$

which is contradiction.

SUBCASE 2.2.2: k is odd.

Distinguish tree subcases:

SUBACSE 2.2.2.1. At least three vertices in C_H are adjacent to vertices in $V(H)\setminus V(C_H)$.

Let these vertices be v_{i_1}, v_{i_2} and v_{i_3}. Denote by w_{i_1}, w_{i_2} and w_{i_3} vertices in $V(H)\setminus V(C_H)$ such that $v_{i_1}w_{i_1}$, $v_{i_2}w_{i_2}$ and $v_{i_3}w_{i_3}$ (note that some of vertices w_{i_1}, w_{i_2} and w_{i_3} may be equal, but this will not affect the proof). It can be easily seen that for each j vertices $v_{i_j+(k-1)/2}$ and $v_{i_j+(k+1)/2}$ are on the same distance from the edge $v_{i_j}w_{i_j}$. Hence, edges $v_{i_j+(k-1)/2}v_{i_j+(k+1)/2}$ contribute at most $(m-2)^2/4$. Therefore,

$$Sz_e(H)=(m-3)\cdot\frac{m(m-2)}{4}+3\frac{(m-2)^2}{4}<(m+2)\cdot(m-2)^2/4.$$

SUBACSE 2.2.2.2. Exactly two vertices in C_H are adjacent to vertices in $V(H)\setminus V(C_H)$.

Denote $v_{i_1}, v_{i_2}, w_{i_1}$ and w_{i_2} as in the proof of the last subcase. Similarly as in the proof of the previous case, it can be shown that edges $v_{i_j+(k-1)/2}v_{i_j+(k+1)/2}$ contribute at most $(m-2)^2/4$ for $j=1,2$.

Without loss of generality, we may assume that $i_1 = 0$ and that $i_2 > k/2$. Note that in this case there is no shortest path connecting vertices in $V(H)\backslash\{v_1, v_2, ..., v_{i_2-1}\}$ passes through vertices v_1, $v_2, \ldots, v_{i_2-1}$. Hence, all distances in graph $H' = H - \{v_1, v_2, ..., v_{i_2-1}\}$ are the same as distances in H.

Also, note that graph H' has the same number of leaves as graph H, i.e. it has no leaves. Also, H' is connected. Hence, there is the shortest cycle $C_{H'}$ in H'. Let us distinguish two subcases:

SUBCASE: 2.2.2.2.1: $C_{H'} = H'$ and H' has odd number of vertices.

Denote in order of their appearance vertices of $C_{H'}$ by $u_0, ..., u_{l-1}$ in such way that $u_0 = v_0$. Then, vertices $u_{(l-1)/2}$ and $u_{(l+1)/2}$ are on the same distance (in H) from the edge $v_0 v_1$, but then edge $u_{(l-1)/2} u_{(l+1)/2}$ contributes at most $(m-2)^2/4$. Therefore, $Sz_e(H) = (m-3)\cdot\frac{m(m-2)}{4} + 3\frac{(m-2)^2}{4} < (m+2)\cdot(m-2)^2/4.$

SUBCASE: 2.2.2.2.2: $C_{H'} \neq H'$ or H' has even number of vertices.

Analogously as above, it can be shown that there is an edge e in H' which is on the same distance from two adjacent edges u' and u'' in H', but since distances in H and H' are the same, we have found the third edge that contributes at most $(m-2)^2/4$ and a contradiction can be obtained as above.

SUBACSE 2.2.2.2.3: Only vertex v_0 in C_H is adjacent to vertices in $V(H)\backslash V(C_H)$.

Note that all edges in $H - (V(C_H)\backslash\{v_0\})$ are on the same distance from $v_{(k-1)/2}$ and $v_{(k+1)/2}$. Since, H has no leaves, there are at least 4 edges in $H - (V(C_H)\backslash\{v_0\})$ hence edge $v_{(k-1)/2} v_{(k+1)/2}$ contributes at most $\frac{(m-5)^2}{4}$, but then:

$$Sz_e(H) = (m-1)\cdot\frac{m(m-2)}{4} + \frac{(m-5)^2}{4} < (m+2)\cdot(m-2)^2/4.$$

5. Acknowledgment

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