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Counterexamples to Conjectures on Graphs with the Greatest Edge–Szeged Index

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Abstract

Recently, it was conjectured by Gutman and Ashrafi that the complete graph K_n has the greatest edge-Szeged index among simple graphs with n vertices. This conjecture turned out to be false, but led Vukičević to conjecture the coefficient 1/15552 of n^6 for the approximate value of the greatest edge-Szeged index. We provide counterexamples to this conjecture.

1 Introduction

Let G = (V, E) be a simple graph. Inspired by the property of Wiener index valid for trees, the Szeged index [1] has been introduced as

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

where $n_u(uv|G)$ is the number of vertices closer to vertex u than to vertex v, and $n_v(uv|G)$ is the number of vertices closer to vertex v than to vertex u. Properties of the Szeged index have been extensively studied (see [2] and more recent papers from this journal [3]-[6]).

The modification of this index has been proposed in [7] as

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

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-604-

where $m_u(uv|G)$ is the number of edges lying closer to vertex u than to vertex v, and $m_v(uv|G)$ is the number of edges closer to vertex v than to vertex u. This index is called the *edge-Szeqed index* and some of its properties have been analyzed in [7, 8, 9, 10].

The problem of determining the n-vertex simple graph with greatest edge-Szeged index appears to be tough. The following conjecture was proposed in [7]:

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

This conjecture was refuted in [8]. It was shown there that the value of the greatest edge-Szeged index among *n*-vertex simple graphs is $\Theta(n^6)$ or, in other words,

 $\lim_{n \to \infty} \log_n \max\{Sz_e(G): G \text{ is a simple graph on } n \text{ vertices}\} = 6,$

and a new conjecture was proposed:

Conjecture 2
$$\lim_{n \to \infty} \frac{\max\{Sz_e(G): G \text{ is a simple graph on } n \text{ vertices}\}}{n^6} = \frac{1}{15552}$$

A relatively complicated class of graphs achieving this limit is described in [8].

Our goal here is to refute this conjecture by describing a set of counterexamples. In short, counterexamples are obtained from a cycle C_5 by expanding each of its vertices into a complete graph. In more detail, let n be a positive integer and let $a_i \in \{\lfloor n/5 \rfloor, \lceil n/5 \rceil\}$ for i = 1, ..., 5, such that $\sum_{i=1}^5 a_i = n$. Let G_n be formed from the union of complete graphs K_{a_1}, \ldots, K_{a_5} by adding an edge between a vertex of K_i and a vertex of K_j whenever $i - j \equiv 1 \pmod{5}$. In total, G_n has n vertices and approximately $3n^2/10$ edges (the actual number of edges depends on the distribution of values $\lfloor n/5 \rfloor, \lceil n/5 \rceil$ among a_1, \ldots, a_5 , but it is irrelevant for calculating the limit in Conjecture 2). As an example, G_{11} is shown in Figure 1.

Let us now estimate the contributions of particular edges to $Sz_e(G_n)$. There are two types of edges in G_n : those connecting vertices in distinct complete graphs and those connecting vertices in the same complete graph K_{a_i} . For easier reading, let $k = \lfloor n/5 \rfloor$.

Suppose first that uv is an edge between vertices from distinct complete graphs and, without loss of generality, suppose that $u \in K_{a_3}$ and $v \in K_{a_4}$. Then the edges between K_{a_1} and K_{a_2} , as well as the edges within K_{a_2} , are closer to u than to v. On the other hand, the edges between K_{a_1} and K_{a_5} , as well as the edges within K_{a_5} , are closer to v -605-



Figure 1: Graph G_{11} .

than to u. The remaining edges have equal distance to both u and v, except for those edges having u or v as one of their end vertices. Therefore,

$$m_u(uv|G) = a_1a_2 + \binom{a_2}{2} + a_2 + (a_3 - 1) + (a_4 - 1) \ge \frac{3}{2}k^2 + \frac{5}{2}k - 2,$$

$$m_v(uv|G) = a_1a_5 + \binom{a_5}{2} + a_5 + (a_4 - 1) + (a_3 - 1) \ge \frac{3}{2}k^2 + \frac{5}{2}k - 2.$$

Next, suppose that uv is an edge between two vertices from the same complete graph. Without loss of generation, suppose that $u, v \in K_{a_3}$. Then all edges have equal distance to both u and v, except for those edges having u or v as one of their end vertices. In this case

$$m_u(uv|G) = m_v(uv|G) = (a_3 - 2) + a_2 + a_4 \ge 3k - 2.$$

We see that the important contribution to $Sz_e(G_n)$ comes from the edges connecting vertices from distinct complete graphs. The number of such edges is $\sum_{i=1}^{5} a_i a_{i+1} \ge 5k^2$, and so we have

$$Sz_e(G_n) \ge 5k^2 \left(\frac{3}{2}k^2 + \frac{5}{2}k - 2\right)^2 > \frac{45}{4}k^6$$

Therefore,

$$\lim_{n \to \infty} \frac{\max\{Sz_e(G): G \text{ is a simple graph on } n \text{ vertices}\}}{n^6}$$
$$\geq \lim_{n \to \infty} \frac{Sz_e(G_n)}{n^6} \geq \lim_{n \to \infty} \frac{\frac{45}{4} \lfloor n/5 \rfloor^6}{n^6} = \frac{45}{4 \cdot 5^6} = \frac{9}{12500} > \frac{1}{15552}$$

So, Conjecture 2 turns out to be false as well.

Although the computer search on up to ten vertices suggests so, we are not entirely convinced that graphs G_n are truly the graphs with greatest edge-Szeged index among *n*-vertex graphs. Due to the nature of the edge-Szeged invariant and the structure of graphs G_n , one would have to search among the graphs with up to 20 vertices in order to get a better understanding of extremal graphs for the edge-Szeged index. This is certainly beyond the reach of present-day computers. In such case, a metaheuristic search may be employed, such as variable neighborhood search, particle sworm optimization or genetic algorithm, although it is not certain that truly extremal graphs will be found that way.

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