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On the discrepancy between two Zagreb indices

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ABSTRACT

We examine the quantity

$$S(G) = \sum_{uv \in E(G)} \min(\deg u, \deg v)$$

over sets of graphs with a fixed number of edges. The main result shows the maximum possible value of $S(G)$ is achieved by three different classes of constructions, depending on the distance between the number of edges and the nearest triangular number. Furthermore we determine the maximum possible value when the set of graphs is restricted to be bipartite, a forest, or to be planar given sufficiently many edges. The quantity $S(G)$ corresponds to the difference between two well studied indices, the irregularity of a graph and the sum of the squares of the degrees in a graph. These are known as the first and third Zagreb indices in the area of mathematical chemistry.

1. Introduction

1.1. The specialty of a graph

The following question appeared on the Team Selection Test for the 2018 United States International Math Olympiad team.

Problem 1. At a university dinner, there are 2017 mathematicians who each order two distinct entrées, with no two mathematicians ordering the same pair of entrées. The cost of each entrée is equal to the number of mathematicians who ordered it, and the university pays for each mathematician's less expensive entrée (ties broken arbitrarily). Over all possible sets of orders, what is the maximum total amount the university could have paid?

This problem, posed by Evan Chen, proved extremely challenging for contestants, with only one full solution given on the contest. We can rephrase the question in more graph theoretic terms.

Definition 2. Define the **specialty** of a graph G to be

$$S(G) = \sum_{uv \in E(G)} \min(\deg u, \deg v)$$

where $E(G)$ is the edge set of a graph G.

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The question posed to the contestants therefore is equivalent to evaluating

$$F(2017) = \max_{G \text{ has } 2017 \text{ edges}} S(G).$$

The given solutions relied heavily on the fact that $2017 = \binom{64}{2} + 1$, and therefore the maximizing graph is near a complete graph. The purpose of this note is to determine

$$F(N) = \max_{G \text{ has } N \text{ edges}} S(G)$$

in general, as well as to determine the maximum when G is further restricted to be bipartite, a forest, or planar given sufficiently many edges in the final case.

1.2. Relation to Zagreb indices

The specialty of a graph is intimately related to two quantities of a graph, the irregularity of a graph and the sum of the squares of the degrees. First, Albertson [4] defines the irregularity of G, which we denote as $M_3(G)$, to be

$$M_3(G) = \sum_{uv \in E(G)} \left| \deg u - \deg v \right|.$$

Fath-Tabar [11] also defines this as the third Zagreb index, hence the choice of notation. Tavakoli and Gutman [22] as well as Abdo, Cohen, and Dimitrov [1] independently determined the maximum of $M_3(G)$ over all graphs with n vertices. For further results regarding irregularity for various classes of graphs see [14,17], and [24].

On the other hand if the minimum of the degrees is replaced with a sum of the degrees in the definition of specialty, the corresponding quantity

$$M_1(G) = \sum_{uv \in E(G)} (\deg u + \deg v) = \sum_{v \in V(G)} (\deg v)^2$$

roughly counts the number of directed paths of length 2 in G. The problem of maximizing this quantity over all graphs with a particular number of edges and vertices was a problem introduced in 1971 by Katz [15]. The first exact results in this problem were given by Ahlswede and Katona who in essence demonstrated that the maximum value is achieved on at least one of two possible graphs called the quasi-complete and quasi-star graphs [3]. However, as Erdős remarked in his review of the paper, "the solution is more difficult than one would expect" [10]. Ábrego, Fernández-Merchant, Neubauer, and Watkins furthered this result by determining the exact maximum in all cases [2]. However, given the complexity of the exact value of the upper bound, there was considerable interest in giving suitable upper bounds and a vast literature of such bounds developed. See [5–8,20,25,23] for many results of this type. Many of these results stem from the area of mathematical chemistry and the above quantity is referred to as the first Zagreb index, $M_1(G)$. In this context, using the notation in [11], we resolve the problem of maximizing

$$\begin{aligned} S(G) &= \frac{1}{2} \sum_{uv \in E(G)} (\deg u + \deg v - |\deg u - \deg v|) \\ &= \frac{M_1(G) - M_3(G)}{2}, \end{aligned}$$

that is, the discrepancy between two of these already-studied graph invariants, over graphs with a fixed number of edges. Note that both $M_1(G)$ and $M_3(G)$ can both trivially have order of the square of the number of edges, and in this paper we in fact show that $S(G)$ has a strictly lower order. Furthermore, the maximum of $S(G)$ being of lower order extends to when G is restricted to be a bipartite graph, a forest, or a planar graph. (The maximum value of $M_1(G)$ over a fixed number of edges is achieved by a star [3]. For $M_3(G)$ the maximum value over the set of all trees is achieved by a star [16] and one can easily check that this extends to all planar graphs.)

1.3. Combinatorial interpretation

We end with an alternate combinatorial interpretation of $S(G)$ arising through the related $S'(G)$ where

$$S'(G) = \frac{1}{3} \sum_{uv \in E(G)} (\min(\deg u, \deg v) - 1) = \frac{1}{3} S(G) - \#E(G).$$

Note that $S'(G)$ provides a trivial upper bound for the number of triangles in a graph G and a solution to the initial problem therefore provides an upper bound for the number of triangles in a graph with a specified number of edges.

Erdős gave a remarkably short proof that for graphs with $N = \binom{n}{2} + m$ edges (with $1 \leq m \leq n$), the maximum number of triangles is achieved on a complete graph with n vertices and an additional vertex connected to m vertices in the clique [9]. The remarkable fact therefore is that the maximum of $S(G)$ is not always achieved on the same graphs as those that maximize the number of triangles, despite the optimal constructions agreeing for infinitely many integers (with a density of $\frac{2}{5}$).