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On the extremal values of general degree-based graph entropies

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ABSTRACT

In this note we prove one part of the conjecture about upper and lower bounds of the degree-based graph entropy $I_k(T)$ in the class of trees introduced in [S. Cao, M. Dehmer, Y. Shi, *Extremality of degree-based graph entropies*, Information Sciences 278 (2014) 22–33.] using Lagrange multipliers and Jensen's inequality, and disprove the other part by providing a family of counter-examples. Our main result is the following: the path P_n is unique tree on n vertices that maximizes $I_k(T)$ for $k > 0$, and the star S_n is unique tree on n vertices that minimizes $I_k(T)$ for $k \geq 1$.

1. Introduction

A variety of problems in many fields, like computer science, information theory or biology, deal with characterizing relational structures by using different graph measures. In this paper we analyze information-theoretic network measures representing graph entropies [5]. It has been proven that these information-theoretic quantities possess useful properties such as a meaningful structural interpretation and uniqueness [4,6,10]. Many graph invariants have been used for the construction of Shannon entropy-based measures to characterize the structure of complex networks [3].

Let G be a simple graph on n vertices and m edges. Let $deg(v)$ denotes the degree of the vertex v. Let P_n and S_n be the path and the star on n vertices, respectively.

Recently Cao, Dehmer and Shi in [2] introduced the following degree-based graph entropy by extending the Shannon's entropy:

$$I_k(G) = \ln\left(\sum_{i=1}^{n} deg(v_i)^k\right) - \frac{1}{\sum_{i=1}^{n} deg(v_i)^k}\sum_{i=1}^{n} deg(v_i)^k \ln\left(deg(v_i)^k\right).$$

The authors mostly analyzed the special case $k = 1$, as the sum of all degree powers is constant and equals $2m$. The main contribution of that paper is proving some extremal values for the underlying graph entropy of certain families of graphs and to find the connection between the graph entropy and the sum of graph degrees power.

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The above index is directly connected to the sum of powers of vertex degrees. The first general Zagreb index [8] is defined as follows:

$$M_k(G) = \sum_{v \in V} deg(v)^k,$$

where $k \in R$. For more information on the Zagreb index and generalizations see [7,8,13,14] and references therein. Li and Zheng [12] proved the following result for the extremal trees with respect to $M_k(G)$. Note that for $k = 0$ or $k = 1$, the values of the first general Zagreb index are constant for all graphs: $M_0(G) = n$ and $M_1(G) = 2m$.

Theorem 1. *Among all trees with n vertices, S_n is the unique extremal tree with the largest general Zagreb index when $k < 0$ or $k > 1$, and the smallest general Zagreb index when $0 < k < 1$.*

Among all trees with n vertices, P_n is the unique extremal tree with the smallest general Zagreb index when $k < 0$ or $k > 1$, and the largest general Zagreb index when $0 < k < 1$.

For better understanding the graph invariants, it is essential to determine the maximal and minimal values in the class of trees on n vertices. Based on numerical experiments, the authors from [2] obtained the following conjecture and stated that "several attempts to prove the statement by using different methods failed".

Conjecture 2. *Let T be a tree with n vertices and $k > 0$. Then we have $I_k(T) \leq I_k(P_n)$, the equality holds if and only if $T \cong P_n$; and $I_k(T) \geq I_k(S_n)$, the equality holds if and only if $T \cong S_n$.*

In order to prove this conjecture, the authors examined various mathematical properties of I_k.

In this paper we prove the above conjecture for $k \geq 1$ using Lagrange multipliers method. For $0 < k < 1$, we disprove the second part of conjecture about S_n by constructing a family of counterexamples for small values of k, and then prove the first part about P_n using Jensen's inequality. We summarize the results in Section 3 and leave the remaining case for the future research.

2. Main result

In this section, we are first going to prove Conjecture 2 using partial derivatives and conditional extremums of multi-variable functions for the case $k \geq 1$. For more details on the Lagrange multipliers see [1,15].

2.1. Case $k \geq 1$

For simplicity, enumerate the vertices from 1 to n, and let $deg(v_i)^k = x_i$. As every tree has at least two leaves, without loss of generality we can assume that $x_{n-1} = x_n = 1^k = 1$. Furthermore, let X be a fixed constant defined as a sum of all remaining coordinates

$$X = \sum_{i=1}^{n-2} deg(v_i)^k = \sum_{i=1}^{n-2} x_i.$$

Also let

$$Y = X + 2 = \sum_{i=1}^{n} deg(v_i)^k = \sum_{i=1}^{n} x_i.$$

We are analyzing conditional extremums of the following function

$$f(x_1, x_2, \ldots, x_{n-2}, 1, 1) = \ln(X+2) - \frac{1}{X+2} \cdot \sum_{i=1}^{n-2} x_i \ln x_i$$

and corresponding Lagrangian function

$$F(x_1, x_2, \ldots, x_{n-2}) = f(x_1, x_2, \ldots, x_{n-2}, 1, 1) + \lambda \left(\sum_{i=1}^{n-2} x_i - X \right),$$

with the additional boundary conditions $x_i \geq 1$. The function is well-defined and differentiable with respect to each of its arguments on the closed region, so the extremal values can be either critical points or on the boundary. By direct calculation, the partial derivatives for each $i = 1, 2, \ldots, n-2$ are equal to:

$$F'_{x_i} = -\frac{1}{X+2}(\ln x_i + 1) + \lambda = 0.$$

From this system of equations it follows that that unique critical point C satisfies $x_1 = x_2 = \ldots = x_{n-2} = e^{\lambda(X+2)-1} = \frac{X}{n-2} > 1$. Furthermore, using the second order conditions it follows that this is a local maximum, as $F''_{x_i} < 0$.