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Degree-based entropies of networks revisited

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ABSTRACT

Studies on the information content of graphs and networks have been initiated in the late fifties based on the seminal work due to Shannon and Rashevsky. Various graph parameters have been used for the construction of entropy-based measures to characterize the structure of complex networks. Based on Shannon's entropy, in Cao et al. (Extremality of degree-based graph entropies, Inform. Sci. 278 (2014) 22–33), we studied graph entropies which are based on vertex degrees by using so-called information functionals. As a matter of fact, there has been very little work to find their extremal values when considered Shannon entropy-based graph measures. We pursue with this line of research by proving further extremal properties of the degree-based graph entropies.

1. Introduction

The four main types of complex networks include weighted digraphs (directed graphs), unweighted digraphs, weighted graphs and unweighted graphs. In this paper, we only consider unweighted undirected graphs.

Studies on the information content of graphs have been initiated in the late fifties inspired by the seminal work due to Shannon [60] and Rashevsky [57]. The concept of graph entropy [17,22] introduced by Rashevsky [57] has been used to measure the structural complexity of graphs [18,19]. The entropy of a graph is an information-theoretic quantity that has been firstly introduced by Mowshowitz [51]. Here the complexity of a graph [23] is based on the well-known Shannon's entropy [12,17,51,50]. Importantly, Mowshowitz interpreted his graph entropy measure as the structural information content of a graph and demonstrated that this quantity satisfies important properties when using product graphs etc, see, e.g., [52–55]. Note the Körner's graph entropy [38] has been introduced from an information theory point of view and has not been used to characterize graphs quantitatively. An extensive overview on graph entropy measures can be found in [22]. A statistical analysis of topological graph measures has been performed by Emmert-Streib and Dehmer [27].

Several graph invariants, such as the number of vertices, the vertex degree sequences, extended degree sequences (i.e., the second neighbor, third neighbor, etc.), Eigenvalues, and connectivity information, have been used for developing entropy-based measures [17,20,22,25–26]. In [10], the authors study novel properties of graph entropies which are based on an information functional by using degree powers of graphs. The degree powers is one of the most important graph invariant, which has been proven useful in information theory, and for studying social networks, network reliability and problems in mathematical chemistry. For more results on properties of degree powers, we refer to [3,4,31–33,41–44,46,48,49,58]. In particular, they

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determine the extremal values for the underlying graph entropy of certain families of graphs and find the connection between graph entropy and the sum of degree powers, which is well-studied in graph theory and some related disciplines.

The main contribution of the paper is to extend the results performed in [10]. In this paper, we explore extremal values of a special graph entropy measure and the relations between this entropy and the sum of degree powers for different values of k. We demonstrate this by generating numerical results using trees with 11 vertices and connected graphs with 7 vertices, respectively, while in [10], some graph transformations are established to find extremal values of entropy for some classes of graphs when $k = 1$. In addition, we also make an effort on finding relations between the values of the graph entropy measure and k.

The paper is organized as follows. In Section 2, some concepts and notation in graph theory are introduced. In Section 3, we introduce some results on the sum of degree powers. In Section 4, we state the definitions of graph entropies based on the given information functional by using degree powers. In Sections 5 and 6, extremal properties of graph entropies have been studied. Further, we express some conjectures to find extremal values of trees.

2. Preliminaries

A *graph* G is an ordered pair of sets $V(G)$ and $E(G)$ such that the elements $uv \in E(G)$ are a sub-collection of the unordered pairs of elements of $V(G)$. For convenience, we denote a graph by $G = (V, E)$ sometimes. The elements of $V(G)$ are called *vertices* and the elements of $E(G)$ are called *edges*. If $e = uv$ is an edge, then we say vertices u and v are *adjacent*, and u, v are two endpoints (or ends) of e. A *loop* is an edge whose two endpoints are the same one. Two edges are called *parallel*, if both edges have the same endpoints. A *simple graph* is a graph containing no loops and parallel edges. If G is a graph with n vertices and m edges, then we say the *order* of G is n and the *size* of G is m. A graph of order n is addressed as an *n-vertex graph*, and a graph of order n and size m is addressed as an *(n, m)-graph*.

A graph is *connected* if, for every partition of its vertex set into two nonempty sets X and Y, there is an edge with one end in X and one end in Y. Otherwise, the graph is *disconnected*. In other words, a graph is *disconnected* if its vertex set can be partitioned into two nonempty subsets X and Y so that no edge has one end in X and one end in Y. A *path graph* is a simple graph whose vertices can be arranged in a linear sequence in such a way that two vertices are adjacent if they are consecutive in the sequence, and are nonadjacent otherwise. Likewise, a *cycle graph* on three or more vertices is a simple graph whose vertices can be arranged in a cyclic sequence in such a way that two vertices are adjacent if they are consecutive in the sequence, and are nonadjacent otherwise. Denote by P_n and C_n the path graph and the cycle graph with n vertices, respectively.

A connected graph without any cycle is a *tree*. Actually, the path P_n is a tree of order n with exactly two pendent vertices. The *star* of order n , denoted by S_n , is the tree with $n - 1$ pendent vertices.

All vertices adjacent to vertex u are called *neighbors* of u. The *neighborhood* of u is the set of the neighbors of u. The number of edges adjacent to vertex u is the *degree* of u, denoted by $d(u)$. Vertices of degrees 0 and 1 are said to be *isolated* and *pendent vertices*, respectively. A pendent vertex is also referred to as a *leaf* of the underlying graph. A vertex of degree i is also addressed as an *i-degree vertex*. The minimum and maximum degree of G is denoted by $\delta(G)$ and $\Delta(G)$, respectively. If G has a_i vertices of degree d_i $(i = 1, 2, \ldots, t)$, where $\Delta(G) = d_1 > d_2 > \cdots > d_t = \delta(G)$ and $\sum_{i=1}^{t} a_i = n$, we define the *degree sequence* of G as $D(G) = [d_1^{a_1}, d_2^{a_2}, \ldots, d_t^{a_t}]$. If $a_i = 1$, we use d_i instead of $d_i^{a_i}$ for convenience.

For terminology and notations not defined here, we refer the reader to [9].

3. Degree-based graph entropies

First, we state the definition of Shannon's entropy [60].

Definition 1. Let $p = (p_1, p_2, \ldots, p_n)$ be a probability vector, namely, $0 \le p_i \le 1$ and $\sum_{i=1}^{n} p_i = 1$. Shannon's entropy of p is defined as

$$I(p) = -\sum_{i=1}^{n} p_i \log p_i.$$

To define information-theoretic graph measures, we will often consider a tuple $(\lambda_1, \lambda_2, \ldots, \lambda_n)$ of non-negative integers $\lambda_i \in \mathbb{N}$ [17]. This tuple forms a probability distribution $p = (p_1, p_2, \ldots, p_n)$, where

$$p_i = \frac{\lambda_i}{\sum_{j=1}^{n} \lambda_j} \qquad i = 1, 2, \ldots, n.$$

Therefore, the entropy of tuple $(\lambda_1, \lambda_2, \ldots, \lambda_n)$ is given by

$$I(\lambda_1, \lambda_2, \ldots, \lambda_n) = -\sum_{i=1}^{n} p_i \log p_i = \log\left(\sum_{i=1}^{n} \lambda_i\right) - \sum_{i=1}^{n} \frac{\lambda_i}{\sum_{j=1}^{n} \lambda_j} \log \lambda_i. \tag{1}$$

In the literature, there are various ways to obtain the tuple $(\lambda_1, \lambda_2, \ldots, \lambda_n)$, like the so-called magnitude-based information measures introduced by Bonchev and Trinajstić [5], or partition-independent graph entropies, introduced by Dehmer [17,24], which are based on information functionals. We are now ready to define the entropy of a graph due to Dehmer [17] by using information functionals.