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Entropy bounds for dendrimers

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ABSTRACT

Many graph invariants have been used for the construction of entropy-based measures to characterize the structure of complex networks. When considering Shannon entropy-based graph measures, there has been very little work to find their extremal values. A reason for this might be the fact that Shannon's entropy represents a multivariate function and all probability values are not equal to zero when considering graph entropies. Dehmer and Kraus proved some extremal results for graph entropies which are based on information functionals and express some conjectures generated by numerical simulations to find extremal values of graph entropies. Dehmer and Kraus discussed the extremal values of entropies for dendrimers. In this paper, we continue to study the extremal values of graph entropy for dendrimers, which has most interesting applications in molecular structure networks, and also in the pharmaceutical and biomedical area. Among all dendrimers with n vertices, we obtain the extremal values of graph entropy based on different well-known information functionals. Numerical experiments verifies our results.

1. Introduction

Exploring graph measures defined on the graph topology has been a fruitful research topic for decades [1–6]. Based on this research, many interdisciplinary areas such as mathematical chemistry, systems biology and mathematical psychology have been influenced when exploring network-based systems quantitatively, see, e.g., [1,7–9]. There are also some results and new techniques to characterize actual networks of contacts, new insights into the problem of how cooperative behavior arises and survives have been provided [10–15]. This is also a new direction for our further research.

Studies of the information content of graphs and networks have been initiated in the late fifties based on the seminal work due to Shannon [16]. The concept of graph entropy [3,17] introduced by Rashevsky [18] and Trucco [19] has been used to measure the structural complexity of graphs [1,20,21]. The entropy of a graph is an information-theoretic quantity that has been introduced by Mowshowitz [22] and he interpreted it as the structural information content of a graph [22–25]. Here the complexity of a graph [26] is based on the well-known Shannon's entropy [27,3,16,22]. Note the Körner's graph entropy [28] has been introduced from an information theory point of view and has not been used to characterize graphs

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quantitatively. A survey on graph entropy measures has been published by Dehmer and Mowshowitz [17]. A statistical analysis of topological graph measures has been performed by Emmert-Streib and Dehmer [29].

In view of the vast of amount of existing graph entropy measures [1,3], there has been very little work to find their extremal values [30]. A reason for this might be the fact that Shannon's entropy represents a multivariate function and all probability values are not equal to zero when considering graph entropies. To the best of our knowledge, Dehmer and Kraus [30] were the first who determined minimal values of graph entropies. Still this problem is intricate because there is a lack of analytical methods to tackle this particular problem. Other related work is due to Shi [31], who proved a lower bound of quantum decision tree complexity by using Shannon's entropy. Dragomir and Goh [32] obtained several general upper bounds for Shannon's entropy by using Jensen's inequality [33].

In [30], Dehmer and Kraus proved some extremal results for graph entropies which are based on information functionals. In particular, they derived information inequalities for dendrimers and statements regarding the extremality of the graph entropy by using majorization theory [34] and several information functionals [17]. Furthermore, they expressed some conjectures generated by numerical simulations to find extremal values of the mentioned graph entropies.

The main contribution of the paper is to prove extremal results for dendrimers. In order to achieve our mathematical results, we employ graph entropies which are based on information functionals (see Section 2). The reason why we study dendrimers is that they have been proven useful in structural chemistry and in the pharmaceutical and biomedical area. For details on the theory of dendrimers, see [35–37].

2. Preliminaries

In the whole paper, "log" denotes the logarithm based on 2. In the following, we introduce entropy measures studied in this paper and state some preliminaries [3,38]. All measures examined in this paper are based on Shannon's entropy.

Definition 1. Let $p = (p_1, p_2, \dots, p_n)$ be a probability vector, namely, $0 \leqslant p_i \leqslant 1$ and $\sum_{i=1}^{n} p_i = 1$. The 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 often consider a tuple $(\lambda_1, \lambda_2, \dots, \lambda_n)$ of non-negative integers $\lambda_i \in \mathbb{N}$ [3]. This tuple forms a probability distribution $p = (p_1, p_2, \dots, p_n)$, where

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

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

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

In the literature, there are various ways to obtain the tuple $(\lambda_1, \lambda_2, \dots, \lambda_n)$, like the so-called magnitude-based information measures introduced by Bonchev and Trinajstić [39], or partition-independent graph entropies, introduced by Dehmer [3,40], which are based on information functionals.

We are now ready to define the entropy of a graph due to Dehmer [3] by using information functionals.

Definition 2. Let $G = (V, E)$ be a undirected connected graph. For a vertex $v_i \in V$, we define

$$p(v_i) := \frac{f(v_i)}{\sum_{j=1}^{|V|} f(v_j)},$$

where f represents an arbitrary information functional.

Observe that $\sum_{i=1}^{|V|} p(v_i) = 1$. Hence, we can interpret the quantities $p(v_i)$ as vertex probabilities. Now we immediately obtain one definition of graph entropy of a graph G.

Definition 3. Let $G = (V, E)$ be a undirected connected graph and f be an arbitrary information functional. The entropy of G is defined as

$$I_f(G) = -\sum_{i=1}^{|V|} \frac{f(v_i)}{\sum_{j=1}^{|V|} f(v_j)} \log\left(\frac{f(v_i)}{\sum_{j=1}^{|V|} f(v_j)}\right) = \log\left(\sum_{i=1}^{|V|} f(v_i)\right) - \sum_{i=1}^{|V|} \frac{f(v_i)}{\sum_{j=1}^{|V|} f(v_j)} \log f(v_i). \tag{2}$$

There is a large number of information functionals which can be used, see [3,17,41,40].

3. Extremal values for graph entropies of dendrimers

A dendrimer is a tree with 2 additional parameters, the progressive degree t and the radius r (as an example, see Fig. 1). Every internal node of the tree has degree $t + 1$. As in every tree, a dendrimer has one (monocentric dendrimer) or two