Generalized Graph Entropies

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Abstract

This paper deals with generalized entropies for graphs. These entropies result from applying information measures to a graph using various schemes for defining probability distributions over the elements (e.g., vertices) of the graph. We introduce a new class of generalized measures, develop their properties, and illustrate the theory with applications to selected graphs.

Key words: Entropy, Graph Entropy, Information Theory, Information Measures

1 Introduction

Studies of the information content of graphs and networks was initiated in the late 1950s following publication of the widely cited paper of Shannon [36] on information and communication. The broad range of research on entropy and graphs is exemplified in [5, 6, 29, 37]. Early contributions (e.g., [25, 33, 38]) in this field inspired researchers (e.g., [6, 15, 29, 40]) to apply entropy measures to problems spanning different disciplines. Now that numerous measures have been developed, it is often difficult to choose a measure suitable for solving a given problem. To choose an appropriate measure it is essential to have a clear idea of the structural feature to be measured in a graph or network. We have addressed this problem in [16, 17]. For additional related work, see [9, 30].

This paper is intended as a contribution to the development of generalized entropy measures on graphs. Although a comprehensive review of the extensive work on generalized entropy measures is beyond the scope of this paper, we offer a brief history of such measures applied to graphs. Classical information measures on graphs can be traced to the work of Trucco [38], Rashevsky [33], and Mowshowitz [29, 26, 27, 28]. These papers defined several related measures based on partitions of the vertices of a graph. Examples of such partitions include the collection of orbits of the automorphism group, and decompositions associated with colorings of a graph. [29, 26].Bonchev et al. [5, 6, 10] generalized these measures by defining weighted probability distributions that yield measures with a higher discrimination power [5, 6, 7, 8]. Related indices for measuring the information content of a network were subsequently explored in [18, 23, 22, 34]. Taking information measures in a new direction, Dehmer [13] developed graph entropies that are not dependent on a partition induced by a graph invariant.

The aim of this paper is to introduce a new class of measures (called here *generalized measures*) that derive from functions such as those defined by Rényi entropy [35] and Daròczy [12]. The innovation represented by these generalized entropy measures is their dependence on the assignment of a probability distribution to a set of elements of a graph. Rather than determine a probability distribution from properties of a graph, one is imposed on the graph independently of its internal structure. Similar (parametric) entropy measures have been used to investigate the complexity of graphs associated with machine learning procedures [14]. Such measures have proved useful in demonstrating that hypotheses can be learned by using appropriate data sets and parameter optimization techniques. In addition, some properties of parametric entropies have already been examined [12, 35]; and results in this area are applicable to generalized graph entropies. A study examining relationships between these parametric graph entropies (see Section (3)) is in progress.

This paper is organized as follows. Section (2) reviews existing entropy measures defined on graphs. In Section (3), we introduce a new class of generalized graph entropy measures and detail some relationships between them. Also, numerical values of the measures are computed for selected graphs and their implications for complexity measurement are discussed. Section (4) offers a short summary and conclusion.

2 Graph Entropies

Here we present two classes of graph entropy measures that play a role in the remainder of the paper. The first class includes classical measures based on an equivalence relation τ defined on the set X of elements of a graph. The relation τ partitions X into equivalence classes and thus allows for defining a probability distribution in a natural way, e.g., [29, 26, 6]. This approach yields a measure of the structural information content of a graph $G = (V, E)$, expressed by [29, 6]:

$$I(G,\tau) = -\sum_{i=1}^{k} \frac{|X_i|}{|X|} \log\left(\frac{|X_i|}{|X|}\right), \tag{1}$$

where

$$p_i := \frac{|X_i|}{|X|}. \tag{2}$$

V is the set of vertices and E is the set of edges, respectively. p_i is the probability of equivalence class X_i, and k is the number of equivalence classes of the relation. As noted above, this type of measure is partition-based, i.e., an equivalence relation is defined relative to a set of graph elements (e.g., vertices, edges, etc.) or properties (e.g., distances, degrees, eigenvalues etc.). Partition-based measures allow for quantifying the structural information of a graph or network, see, e.g., [29, 26, 3, 6, 10].

The second class of information measures, introduced by Dehmer [13], is not based on partitions induced by equivalence relations. For the measures in this class an arbitrary probability distribution is associated with the vertices of a graph. By assigning a probability to each vertex $v_i \in V$, we obtain the following probability distribution

$$(p(v_1), p(v_2), \ldots, p(v_n)), \quad |V| := n, \tag{3}$$

where

$$p^f(v_i) := \frac{f(v_i)}{\sum_{j=1}^{n} f(v_j)}. \tag{4}$$

and f is an information function mapping graph elements (e.g., vertices) to the non-negative reals. A characteristic feature of f is that it can be used to weight structural features of a graph, see [15]. Finally, the entropy of the underlying graph topology is

$$I_f(G) := -\sum_{i=1}^{n} \frac{f(v_i)}{\sum_{j=1}^{n} f(v_j)} \log\left(\frac{f(v_i)}{\sum_{j=1}^{n} f(v_j)}\right). \tag{5}$$

3 Generalized Graph Entropies

Following the seminal paper of Shannon [36], many generalizations of the entropy measure have been proposed [1, 12, 35]. An important example of such a measure is called the Rényi entropy [35] and is defined by

$$I_\alpha^r(P) := \frac{1}{1-\alpha} \log\left(\sum_{i=1}^{n} (p_i)^\alpha\right), \quad \alpha \neq 1, \tag{6}$$

where $P := (p_1, p_2, \ldots, p_n)$. The limiting value for $\alpha \longrightarrow 1$ yields Shannon entropy as a special case. A useful feature of Rényi entropy is that by judicious choice of the parameter α, particular measures can be specified that differ in the weights assigned to values in their respective probability distributions. For example, if $\alpha > 1$, higher probability values are weighted more heavily than lower values. If $\alpha < 1$, the converse obtains, i.e., lower probability values are weighted more heavily than higher values. For further discussion of the properties of Rényi entropy, see [2]. Rényi and other general entropy functions allow for specifying families of information measures that can be applied to graphs. Like some generalized information measures that have been investigated in information theory [19], we call these families *generalized graph entropies*.

Definition 3.1 *Let G be a graph. Then,*

$$I^1_\alpha(G) := \frac{1}{1-\alpha}\log\left(\sum_{i=1}^{k}\left(\frac{|X_i|}{|X|}\right)^\alpha\right), \quad \alpha \neq 1, \tag{7}$$

and

$$I^2_\alpha(G) := \frac{1}{1-\alpha}\log\left(\sum_{i=1}^{n}\left(\frac{f(v_i)}{\sum_{j=1}^{n} f(v_j)}\right)^\alpha\right), \quad \alpha \neq 1. \tag{8}$$

From Daròczy's entropy [12], we obtain

Definition 3.2 *Let G be a graph. Then,*

$$I^3_\alpha(G) := \frac{\sum_{i=1}^{k}\left(\frac{|X_i|}{|X|}\right)^\alpha - 1}{2^{1-\alpha}-1}, \quad \alpha \neq 1, \tag{9}$$

and

$$I^4_\alpha(G) := \frac{\sum_{i=1}^{n}\left(\frac{f(v_i)}{\sum_{j=1}^{n} f(v_j)}\right)^\alpha - 1}{2^{1-\alpha}-1}, \quad \alpha \neq 1. \tag{10}$$

Following [2], we establish the following connections between the generalized graph entropies:

$$I^1_\alpha(G) = \frac{1}{1-\alpha}\log\left[(2^{1-\alpha}-1)I^3_\alpha(G)+1\right], \tag{11}$$

$$I^2_\alpha(G) = \frac{1}{1-\alpha}\log\left[(2^{1-\alpha}-1)I^4_\alpha(G)+1\right]. \tag{12}$$

As shown below, another generalized graph entropy can be obtained by applying the quadratic entropy function discussed by Arndt [2].

Definition 3.3 *Let G be a graph. Then,*

$$I^5(G) := \sum_{i=1}^{k}\frac{|X_i|}{|X|}\left[1-\frac{|X_i|}{|X|}\right], \tag{13}$$

and

$$I^6(G) := \sum_{i=1}^{n} \frac{f(v_i)}{\sum_{j=1}^{n} f(v_j)} \left[1 - \frac{f(v_i)}{\sum_{j=1}^{n} f(v_j)}\right]. \qquad (14)$$

Based on the relations presented in [2], it is clear that

$$I^5(G) = 1 - e^{-I_2^1(G)}, \quad \alpha = 2, \qquad (15)$$

$$I^6(G) = 1 - e^{-I_2^2(G)}, \quad \alpha = 2. \qquad (16)$$

Now let's discuss some simple properties of the generalized graph entropies based on Rényi's entropy. Since, we stated some relationships between the other entropies (Daròczy's entropy and quadratic entropy) and $I_\alpha^r(P)$, it suffices to put the emphasis on Rényi's entropy. By using Equation (6), we obtain

$$I_\alpha^r\left(\frac{1}{n}, \frac{1}{n}, \ldots, \frac{1}{n}\right) = \log(n), \qquad (17)$$

i.e., maximum entropy. For instance, let $\mathcal{G}_k$ the set of k-regular graphs [21]. Then, it can be easily shown that for all $G \in \mathcal{G}_k$, the vertex probabilities (see Equation (4)) using the information function given by Equation (31) (and many others) are $p^{f_1}(v_i) = \frac{1}{n}$. Hence,

$$I_\alpha^r\left(\frac{1}{n}, \frac{1}{n}, \ldots, \frac{1}{n}\right) = I_\alpha^2(G) = \log(n), \quad \forall G \in \mathcal{G}_k. \qquad (18)$$

Equally, if we denote $\mathcal{G}_I$ to be the set of so-called identity graphs [21] (asymmetric graphs), we infer that $G \in \mathcal{G}_I$ only possesses vertex orbits representing singleton sets, i.e., $|V_i| = 1$. If $|V| := n$, we yield

$$I_\alpha^r\left(\frac{1}{n}, \frac{1}{n}, \ldots, \frac{1}{n}\right) = I_\alpha^1(G) = \log(n), \quad \forall G \in \mathcal{G}_I. \qquad (19)$$

For vertex-transitive graphs, we get $I_\alpha^1(G) = 0$. Finally, values of Daròczy's entropy and the quadratic entropy can be obtained by using the Equations (11), (12), (15), (16). Another important issue would be to explore relations between the probabilities within a family. We won't tackle this problem here and refer to some related work dealing with inferring information inequalities [13, 16]. In [13, 16], relations between vertex probabilities using the information function approach have been established to derive implicit bounds for the resulting entropies. The underlying mathematical apparatus could be used to derive connections between generalized graph entropies. Note that further generalized entropies can be derived by using parametric information measures such as R-norm entropy [4] and the information energy developed by Onicescu [31]. Note that one could derive entirely new information-theoretic distance measures (e.g., generalizations of the Kullback-Leibler distance [24]) for graphs. Useful sources for such derivations may be found in [1, 2, 39, 32]. However, these measures are beyond the scope of this paper.

In what follows we provide a concrete example for each of the measures defined. We need to specify graph invariants to determine a probability distribution (see Equation (2), (4)). Two such invariants are used here, i.e., the spectrum and the automorphism group of a graph. We include these two because they have been investigated extensively. See Cvetkovic et al. [11] for discussion of the graph spectrum invariant, and [29] for the automorphism group invariant. Other invariants like distances, degrees, paths could be also chosen [17]. As explained above, the role of an invariant in information measures is to partition a graph invariant X into equivalence classes X_i, $1 \leq i \leq k$. By choosing the vertex set V of G, one needs to derive classes of topologically equivalent vertices which are called the vertex orbits [29].

Example 3.1 *Let G be an undirected graph and A its adjacency matrix. U is the unity matrix. $P(\lambda) := \det(A - \lambda U)$ is the characteristic polynomial and $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of G. If $f := |\lambda_i|$, then*

$$p^f(v_i) = \frac{|\lambda_i|}{\sum_{j=1}^{n} |\lambda_j|}. \tag{20}$$

Thus, the generalized graph entropies are

$$^{\lambda}I_\alpha^2(G) = \frac{1}{1-\alpha} \sum_{i=1}^{n} \left(\frac{|\lambda_i|}{\sum_{j=1}^{n} |\lambda_j|} \right)^\alpha, \quad \alpha \neq 1, \tag{21}$$

$$^{\lambda}I_\alpha^4(G) = \frac{\sum_{i=1}^{n} \left(\frac{|\lambda_i|}{\sum_{j=1}^{n} |\lambda_j|} \right)^\alpha - 1}{2^{1-\alpha} - 1}, \quad \alpha \neq 1, \tag{22}$$

$$^{\lambda}I^6(G) = \sum_{i=1}^{n} \frac{|\lambda_i|}{\sum_{j=1}^{n} |\lambda_j|} \left[1 - \frac{|\lambda_i|}{\sum_{j=1}^{n} |\lambda_j|} \right]. \tag{23}$$

Now denote the collection of orbits be denoted by

$$S := \{V_1, V_2, \ldots, V_k\}, \tag{24}$$

and their respective probabilities by

$$\frac{|V_1|}{n}, \frac{|V_2|}{n}, \ldots, \frac{|V_k|}{n}, \tag{25}$$

where k is the number of orbits. Then, we derive another class of generalized

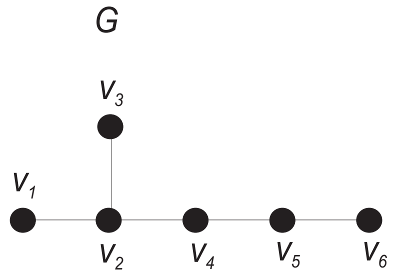

Figure 1: A path graph with one single branch.

graph entropies as

$$I^1_\alpha(G) = \frac{1}{1-\alpha}\log\left(\sum_{i=1}^{k}\left(\frac{|V_i|}{n}\right)^\alpha\right), \quad \alpha \neq 1, \tag{26}$$

$$I^3_\alpha(G) = \frac{\sum_{i=1}^{k}\left(\frac{|V_i|}{n}\right)^\alpha - 1}{2^{1-\alpha}-1}, \quad \alpha \neq 1, \tag{27}$$

$$I^5(G) = \sum_{i=1}^{k}\frac{|V_i|}{n}\left[1 - \frac{|V_i|}{n}\right]. \tag{28}$$

3.1 Numerical Results

In this section, we calculate some of the proposed generalized entropies for the graph G in Figure (1) and plot the results. To calculate these measures in general, we need an information function as well as an equivalence relation to determine probabilities. Starting with I^1_α and I^3_α, we determine the vertex orbits V_i for G explicitly. Thus, we get the probability for each orbit and obtain,

$$\{v_1, v_3\}, \{v_2\}, \{v_4\}, \{v_5\}, \{v_6\}. \tag{29}$$

Hence, $n = 6$ and

$$\frac{|V_1|}{6} = \frac{2}{6}, \frac{|V_2|}{6} = \cdots = \frac{|V_5|}{6} = \frac{1}{6}. \tag{30}$$

To determine I^2_α and I^4_α, we choose the information functions [15]

$$f_1(v_i) := c_1|S_1(v_i,G)| + c_2|S_2(v_i,G)| + \cdots + c_{\rho(G)}|S_{\rho(G)}(v_i,G)|,$$
$$c_k > 0, 1 \leq k \leq \rho(G), \tag{31}$$

and

$$f_2(v_i) := \alpha^{c_1|S_1(v_i,G)| + c_2|S_2(v_i,G)| + \cdots + c_{\rho(G)}|S_{\rho(G)}(v_i,G)|},$$
$$c_k > 0, 1 \leq k \leq \rho(G), \alpha > 0. \tag{32}$$

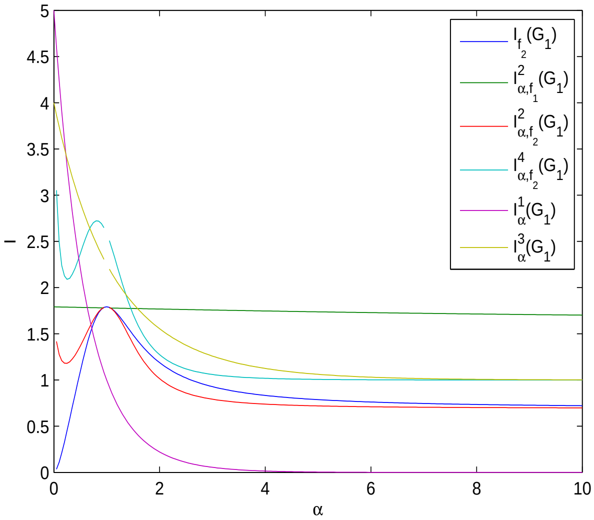

Figure 2: Plotted generalized graph entropies in dependence of α.

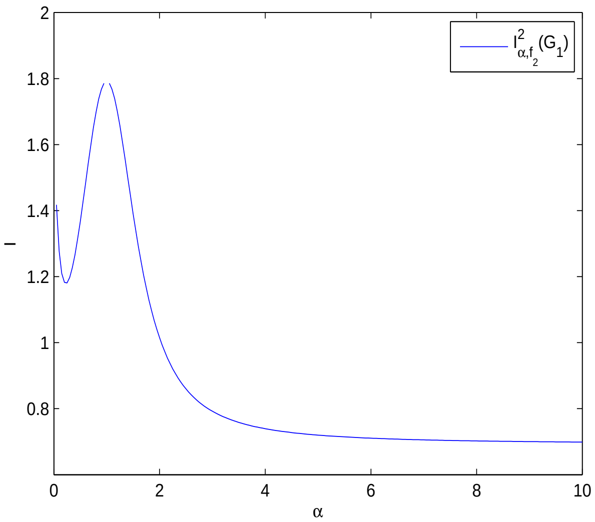

Figure 3: I^2_{α,f_2} in dependence of α with a pole at $\alpha = 1$.

Using f_1, we obtain the following vertex probabilities:

$$p(v_1) = \frac{17}{86} = p(v_2),\ p(v_3) = \frac{15}{86},\ p(v_4) = \frac{13}{86} = p(v_5),\ p(v_6) = \frac{11}{86}. \tag{33}$$

Applying f_2,we get

$$p(v_1) = p(v_2) = \frac{\alpha^{17}}{2\alpha^{17} + \alpha^{15} + 2\alpha^{13} + \alpha^{11}}, \tag{34}$$

$$p(v_3) = \frac{\alpha^{15}}{2\alpha^{17} + \alpha^{15} + 2\alpha^{13} + \alpha^{11}}, \tag{35}$$

$$p(v_4) = p(v_5) = \frac{\alpha^{13}}{2\alpha^{17} + \alpha^{15} + 2\alpha^{13} + \alpha^{11}}, \tag{36}$$

$$p(v_6) = \frac{\alpha^{11}}{2\alpha^{17} + \alpha^{15} + 2\alpha^{13} + \alpha^{11}}. \tag{37}$$

Here, $|S_j(v_i, G)|$ denotes the cardinality of the j-sphere of vertex $v_i \in V$. The meaning of the parameters has been explained in [15]. Turning to Figure (2), we see the plotted values of the entropy measures relative to α. Note that I_{f_1} does not represent a generalized entropy; it is a graph entropy based on Equation (5) using f_1. I^2_{α,f_2} and I^4_{α,f_2} appear to be similar to I_{f_1} since the information function f_2 also depends on the parameter α. [15] has shown that I_{f_1} always has a maximum at $\alpha = 1$. But we see that the curves representing I^2_{α,f_2} and I^4_{α,f_2} have a local minimum as well. It is evident that the generalized measures I^2_{α,f_2} and I^4_{α,f_2} possess poles at $\alpha = 1$, see Figure (2) and Figure (3). This holds as well for I^3_α. By contrast, I^2_{α,f_1} represents a nearly linear curve. The different appearance of I^2_{α,f_1} and I^2_{α,f_2} can be understood by the fact that f_2 is parameterized by α too. Then, by employing the Rényi entropy (in α) leads to strong non-monotonic appearance of the curve I^2_{α,f_2}. Moreover, the generalized entropies I^1_α and I^3_α look rather different because they are not based on vertex probabilities depending on an additional parameter.

4 Summary and Conclusion

In this paper we introduced generalized graph entropies based on existing (parametric) information measures. The starting point was the Rényi entropy [35] from which we derived two types of generalized graph entropy measures. These measures differ according to the probability scheme, Equation (2) and Equation (4), used in their respective definitions. The same procedure was followed for Daròczy's entropy [12]. Figure (2) and Figure (3) give an intuitive idea of the complexity of such measures. In the future, we will perform further numerical studies to evaluate these generalized graph entropies on different graph classes. This can lead to additional insights how these measures behave and how facts Figure (2) might be generalized.

We have not investigated the interrelations between the information measures discussed in this paper by means of inequalities. Given the large number of different information measures that have been defined over the past fifty years, [6, 19, 37], a comprehensive study of interrelations would be a very challenging task. As well as establishing functional interrelations, it is necessary to determine the structural features of the graphs and networks captured by each of the measures. A two-pronged effort seems required: 1) obtain numerical values for a variety of graphs for each of the measures, and 2) derive inequalities between pairs of measures.

As mentioned earlier, parametric complexity measures have proved useful in studies of complexity associated with machine learning. In particular, Dehmer et al. [14] have shown that generalized graph entropies can be applied to problems in machine learning such as graph classification and clustering. These applications involve optimizing certain parameters associated with graphs in a given set (e.g., networks whose graphs are labelled by class tags). A particular set of graphs which has been used extensively in bioinformatics and drug design is given by the database AG 3982 [14, 20] containing two classes of chemical compounds indicating the genetoxicity of a chemical structure. By employing supervised machine learning methods, the new generalized entropies can be used to classify the underlying structures according to optimal values of relevant parameters.

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