Recent Developments in Quantitative Graph Theory: Information Inequalities for Networks

Matthias Dehmer*, **Lavanya Sivakumar**

Institute for Bioinformatics and Translational Research, UMIT, Hall in Tyrol, Austria

Abstract

In this article, we tackle a challenging problem in quantitative graph theory. We establish relations between graph entropy measures representing the structural information content of networks. In particular, we prove formal relations between quantitative network measures based on Shannon's entropy to study the relatedness of those measures. In order to establish such information inequalities for graphs, we focus on graph entropy measures based on information functionals. To prove such relations, we use known graph classes whose instances have been proven useful in various scientific areas. Our results extend the foregoing work on information inequalities for graphs.

Citation: Dehmer M, Sivakumar L (2012) Recent Developments in Quantitative Graph Theory: Information Inequalities for Networks. PLoS ONE 7(2): e31395. doi:10.1371/journal.pone.0031395

Editor: Frank Emmert-Streib, Queen's University Belfast, United Kingdom

Received December 2, 2011; **Accepted** January 6, 2012; **Published** February 15, 2012

Funding: Matthias Dehmer and Lavanya Sivakumar thank the Austrian Science Fund (Project No. PN22029-N13) for supporting this work. The funders had no role in study design, data collection and analysis, decision to publish, or preparation of the manuscript.

Competing Interests: The authors have declared that no competing interests exist.

* E-mail: matthias.dehmer@umit.at

Introduction

Complexity is an intricate and versatile concept that is associated with the design and configuration of any system [1,2]. For example, complexity can be measured and characterized by quantitative measures often called indices [3–5]. When studying the concept of complexity, information theory has been playing a pioneering and leading role. Prominent examples are the theory of communication and applied physics where the famous Shannon entropy [6] has extensively been used. To study issues of complexity in natural sciences and, in particular, the influence and use of information theory, see [7].

In this paper, we deal with an important aspect when studying the complexity of network-based systems. In particular, we establish relations between information-theoretic complexity measures [3,8–11]. Recall that such entropic measures have been used to quantify the information content of the underlying networks [8,12]. Generally, this relates to exploring the complexity of a graph by taking its structural features into account. Note that numerous measures have been developed to study the structural complexity of graphs [5,8,13–22]. Further, the use and ability of the measures has been demonstrated by solving interdisciplinary problems. As a result, such studies have led to a vast number of contributions dealing with the analysis of complex systems by means of information-theoretic measures, see, e.g., [8,13–22]. Figure 1 shows a classification scheme of quantitative network measures exemplarily.

The main contribution of this paper is to study relations between entropy measures. We will tackle this problem by means of inequalities involving network information measures. In particular, we study so-called *implicit information inequalities* which have been introduced by Dehmer et al. [23,24] for studying graph entropies using information functionals. Generally, an implicit information inequality involves information measures which are present on either side of the inequality. It is important to emphasize that relatively little work has been done to investigate relations between network measures. A classical contribution in this area is due to Bonchev et al. [25]. Here, the relatedness between information-theoretic network measures has been investigated to detect branching in chemical networks. Further, implicit information inequalities have been studied for hierarchical graphs which turned out to be useful in network biology [26].

We first present closed form expressions of graph entropies using the graph classes, stars and path graphs. Further, we infer novel information inequalities for the measures based on the j-sphere functional. The section "Implicit Information Inequalities" presents our main results on novel implicit inequalities for networks. We conclude the paper with a summary and some open problems. Before discussing our results, we will first present the information-theoretic measures that we want to investigate in this paper.

Methods

In this section, we briefly state the concrete definitions of the information-theoretic complexity measures that are used for characterizing complex network structures [3,6,9,27]. Here we state measures based on two major classifications namely partition-based and partition-independent measures and deal mainly with the latter.

Given a simple, undirected graph $G=(V,E)$, let $d(u,v)$ denote the distance between two vertices u and v, and let $\rho(G)=\max\{d(u,v):u,v\in V\}$. Let $S_j(u;G)$ denote the j-sphere of a vertex u defined as $S_j(u;G)=\{x\in V:d(u,x)=j\}$. Throughout this article, a graph G represents a simple undirected graph.

Definition 1 *Let $G=(V,E)$ be a graph on n vertices and let X be a graph invariant of G. Let α be an equivalence relation that partitions X into k subsets $X_1,X_2,\dots X_k$, with cardinality $|X_i|$ for $1\leq i\leq k$. The total*

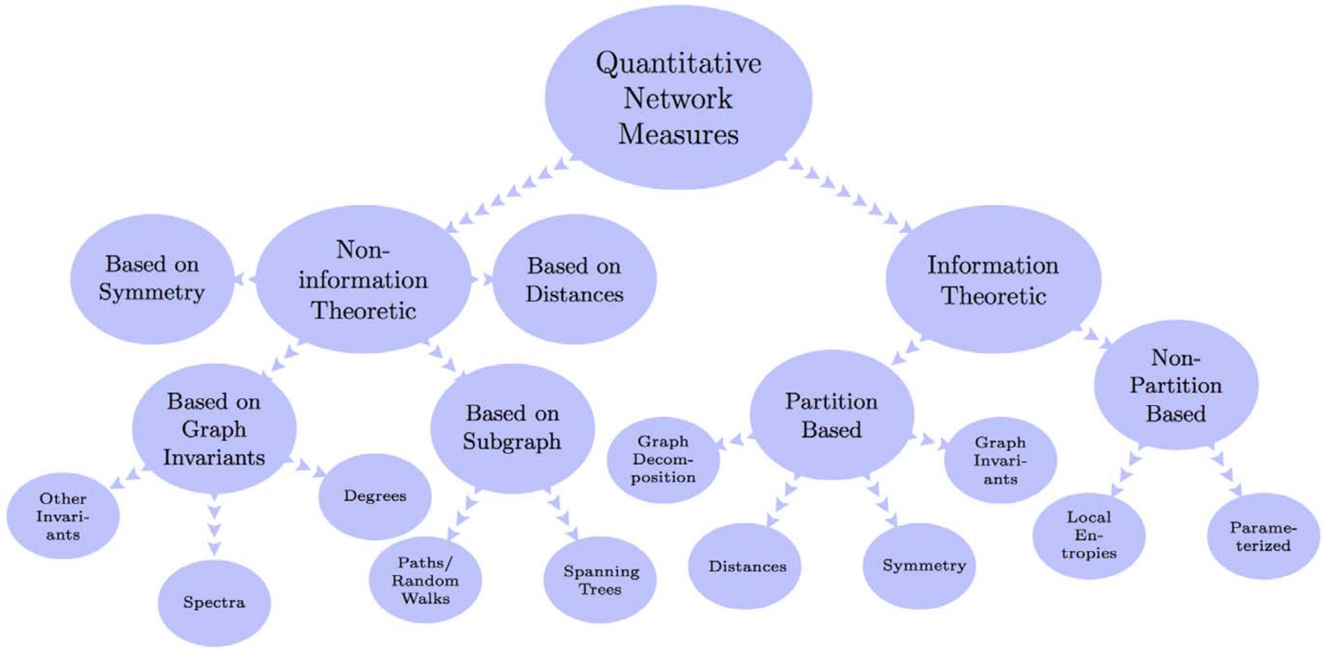

Figure 1. A classification of quantitative network measures.
doi:10.1371/journal.pone.0031395.g001

structural information content of G is given by

$$I_t(G)=|X|\log_2|X|-\sum_{i=1}^{k}|X_i|\log_2|X_i|. \tag{1}$$

Definition 2 *Let $G=(V,E)$ be a graph on n vertices and let $p_i=|X_i|/|X|$, for $1\leq i\leq k$ be the probability value for each partition. The mean information content of G is*

$$I_m(G)=-\sum_{i=1}^{k}p_i\log_2 p_i=-\sum_{i=1}^{k}\frac{|X_i|}{|X|}\log_2\frac{|X_i|}{|X|}. \tag{2}$$

In the context of theory of communication, the above equation is called as Shannon equation of information [28].

Definition 3 *Let $G=(V,E)$ be a graph on n vertices. The quantity*

$$p(v_i)=\frac{f(v_i)}{\sum_{j=1}^{n}f(v_j)}, \tag{3}$$

is a probability value of $v_i\in V$. $f:V\rightarrow R^+$ is an arbitrary information functional that maps a set of vertices to the non-negative real numbers.

Remark 1 *Observe that, $p(\cdot)$ defines a probability distribution over the set of vertices as it satisfies $0\leq p(v_i)<1$, for every vertex v_i, $1\leq i\leq n$ and $\sum_{i=1}^{n}p(v_i)=1$.*

Using the resulting probability distribution associated with G leads to families of network information measures [3,9].

Definition 4 *The graph entropy of G given representing its structural information content:*

$$I_f(G)=-\sum_{i=1}^{n}p(v_i)\log_2 p(v_i)=-\sum_{i=1}^{n}\frac{f(v_i)}{\sum_{j=1}^{n}f(v_j)}\log_2\left(\frac{f(v_i)}{\sum_{j=1}^{n}f(v_j)}\right). \tag{4}$$

In order to define concrete graph entropies, we reproduce the definitions of some information functionals based on metrical properties of graphs [3,9,27].

Definition 5 *Parameterized exponential information functional using j-spheres:*

$$f_P(v_i)=\alpha^{\sum_{j=1}^{\rho(G)}c_j|S_j(v_i;G)|}, \tag{5}$$

where $\alpha>0$ and $c_k>0$ for $1\leq k\leq\rho(G)$.

Definition 6 *Parameterized linear information functional using j-spheres:*

$$f'_P(v_i)=\sum_{j=1}^{n}c_j|S_j(v_i;G)|, \tag{6}$$

where $c_k>0$ for $1\leq k\leq\rho(G)$.

Remark 2 *Observe that, when either $\alpha=1$ or the c_k are all equal, the functional f_P and $f_{P'}$ becomes a constant function and, hence, the probability on all the vertices are equal. That is $p_f(v)=\frac{1}{n}$, for $v\in V$. Thus, the value of the entropy attains its maximum value, $I_f(G)=\log_2(n)$. Thus, in all our proofs, we only consider the non-trivial case, namely $\alpha\neq1$ and/or at least for two coefficients holds $c_j\neq c_k$.*

Next, we will define the local information graph to use local centrality measures from [9]. Let $L_G(v,j)$ be the subgraph induced by the shortest path starting from the vertex v to all the vertices at distance j in G. Then, $L_G(v;j)$ is called the *local information graph regarding v with respect to j*, see [9]. A local centrality measure that can be applied to determine the structural information content of a network [9] is then defined as follows.

Definition 7 *The closeness centrality of the local information graph is defined by*

$$\beta(v;L_G(v,j))=\frac{1}{\sum_{x\in L_G(v,j)}d(v,x)}. \tag{7}$$

Remark 3 *Note that centrality is an important concept that has been introduced for analyzing social networks [29,30]. Many centrality measures* *have been contributed* [30], *and in particular, various definitions for closeness centrality* [30–32]. *We remark that the above definition has been firstly defined by Sabidussi* [31] *for arbitrary graphs. However, we use the measure as a local invariant defined on the subgraphs induced by the local information graph* [9].

Similar to the *j*-sphere functionals, we define further functionals based on the local centrality measure as follows.

Definition 8 *Parameterized exponential information functional using local centrality measure:*

$$f_C(v_i) = \alpha^{\sum_{j=1}^{n} c_j \beta(v_i; L_G(v_i,j))}, \tag{8}$$

where $\alpha > 0$, $c_k > 0$ for $1 \leq k \leq \rho(G)$.

Definition 9 *Parameterized linear information functional using local centrality measure:*

$$f'_C(v_i) = \sum_{j=1}^{n} c_j \beta(v_i; L_G(v_i,j)), \tag{9}$$

where $c_k > 0$, for $1 \leq k \leq \rho(G)$.

Note that the coefficients c_k can be chosen arbitrarily. However, the functionals become more meaningful when we choose the coefficients to emphasize certain structural characteristics of the underlying graphs. Also, this remark implies that the notion of graph entropy is not unique because each measure takes different structural features into account. Further, this can be understood by the fact that a vast number of entropy measures have been developed so far. Importantly, we point out that the measures we explore in this paper are notably different to the notion of graph entropy introduced by Körner [21]. The graph entropy due to Körner [21] is rooted in information theory and based on the known stable set problem. To study more related work, survey papers on graph entropy measures have been authored by Dehmer et al. [3] and Simonyi [33].

Results and Discussion

Closed Form Expressions and Explicit Information Inequalities

When calculating the structural information content of graphs, it is evident that the determination of closed form expressions using arbitrary networks is critical. In this section, we consider simple graphs namely trees with smallest and largest diameter and compute the measures defined in the previous section. By using arbitrary connected graphs, we also derive explicit information inequalities using the measures based on information functionals (stated in the previous section).

Stars. Star graphs, $S(n)$, have been of considerable interest because they represent trees with smallest possible diameter ($\rho(S(n)) = 2$) among all trees on n vertices.

Now, we present closed form expressions for the graph entropy by using star graphs. For this, we apply the information-theoretic measures based on information functionals defined in the preliminaries section.

Theorem 4 *Let* $S(n)$ *be a star on* n *vertices. Let* $f \in \{f_P, f'_P, f_C, f'_C\}$ *be the information functionals as defined before. The information measure is given by*

$$I_f(S(n)) = -x \log_2 x - (1-x) \log_2 \left(\frac{1-x}{n-1}\right), \tag{10}$$

where x *is the probability of the central vertex of* $S(n)$*:*

$$x = \frac{1}{1+(n-1)\alpha^{(c_2-c_1)(n-2)}}, \tag{11}$$

if $f = f_P$.

$$x = \frac{c_1}{2c_1 + c_2(n-2)}, \tag{12}$$

if $f = f'_P$.

$$x = \frac{1}{1+(n-1)\alpha^{c_1\left(\frac{n-2}{n-1}\right)+c_2\left(\frac{1}{2n-3}\right)}}, \tag{13}$$

if $f = f_C$.

$$x = \frac{c_1}{c_1(1+(n-1)^2) + c_2\left(\frac{(n-1)^2}{2n-3}\right)}, \tag{14}$$

if $f = f'_C$.

Proof:

- Consider $f(v) = f_P(v) = \alpha^{\sum_{j=1}^{\rho(S(n))} c_j |S_j(v;S(n))|}$, where $\alpha > 0$ and $c_k > 0$ for $1 \leq k \leq \rho(S(n))$.

We get,

$$f(v) = \begin{cases} \alpha^{c_1(n-1)}, & \text{if } v \text{ is the central vertex,} \\ \alpha^{c_1+c_2(n-2)}, & \text{otherwise.} \end{cases} \tag{15}$$

Therefore,

$$\sum_{v \in V(S(n))} f(v) = \alpha^{c_1(n-1)}\left[1+(n-1)\alpha^{(c_2-c_1)(n-2)}\right]. \tag{16}$$

Hence,

$$p_f(v) = \begin{cases} \dfrac{1}{1+(n-1)\alpha^{(c_2-c_1)(n-2)}}, & \text{if } v \text{ is the central vertex,} \\ \dfrac{\alpha^{(c_2-c_1)(n-2)}}{1+(n-1)\alpha^{(c_2-c_1)(n-2)}}, & \text{otherwise.} \end{cases} \tag{17}$$

By substituting the value of $p_f(v)$ in $I_f(S(n))$ and simplifying, we get

$$I_f(S(n)) = -x \log_2 x - (1-x) \log_2 \left(\frac{1-x}{n-1}\right),$$
$$x = \frac{1}{1+(n-1)\alpha^{(c_2-c_1)(n-2)}}.$$

- Consider $f(v) = f'_P(v) = \sum_{j=1}^{\rho(S(n))} c_j |S_j(v; S(n))|$, where $c_k > 0$ for $1 \leq k \leq \rho(S(n))$.

We get,

$$f(v) = \begin{cases} c_1(n-1), & \text{if } v \text{ is the central vertex,} \\ c_1 + c_2(n-2), & \text{otherwise.} \end{cases} \tag{18}$$

Therefore,

$$\sum_{v\in V(S(n))} f(v)=(n-1)[2c_1+c_2(n-2)]. \tag{19}$$

Hence,

$$p_f(v)=\begin{cases}\dfrac{c_1}{2c_1+c_2(n-2)}, & \text{if } v \text{ is the central vertex,}\\ \dfrac{c_1+c_2(n-2)}{(n-1)[2c_1+c_2(n-2)]}, & \text{otherwise.}\end{cases} \tag{20}$$

By substituting the value of $p_f(v)$ in $I_f(S(n))$ and simplifying, we get

$$I_f(S(n))=-x\log_2 x-(1-x)\log_2\left(\frac{1-x}{n-1}\right),\ x=\frac{c_1}{2c_1+c_2(n-2)}.$$

- Consider the case $f(v)=f_C(v)=\alpha^{\sum_{j=1}^{n} c_j\beta(v;L_{S(n)}(v,j))}$, where $\alpha>0$, $c_k>0$ for $1\leq k\leq \rho(S(n))$.

$$\beta(v;L_{S(n)}(v,j))=\frac{1}{\sum\limits_{x\in L_{S(n)}(v,j)} d(v,x)}, \tag{21}$$

denotes the closeness centrality measure.

Then, we yield

$$f(v)=\begin{cases}\alpha^{c_1(\frac{1}{n-1})}, & \text{if } v \text{ is the central vertex,}\\ \alpha^{c_1+c_2(\frac{1}{2n-3})}, & \text{otherwise.}\end{cases} \tag{22}$$

Therefore,

$$\sum_{v\in V(S(n))} f(v)=\alpha^{c_1(\frac{1}{n-1})}+(n-1)\alpha^{c_1+c_2(\frac{1}{2n-3})}. \tag{23}$$

Hence,

$$p_f(v)=\begin{cases}\dfrac{1}{1+(n-1)\alpha^{c_1(\frac{n-2}{n-1})+c_2(\frac{1}{2n-3})}}, & \text{if } v \text{ is the central vertex,}\\ \dfrac{\alpha^{c_1(\frac{n-2}{n-1})+c_2(\frac{1}{2n-3})}}{1+(n-1)\alpha^{c_1(\frac{n-2}{n-1})+c_2(\frac{1}{2n-3})}}, & \text{otherwise.}\end{cases} \tag{24}$$

By substituting the value of $p_f(v)$ in $I_f(S(n))$ and simplifying, we obtain

$$I_f(S(n))=-x\log_2 x-(1-x)\log_2\left(\frac{1-x}{n-1}\right).$$

where $x=\dfrac{1}{1+(n-1)\alpha^{c_1(\frac{n-2}{n-1})+c_2(\frac{1}{2n-3})}}$.

- Consider $f(v)=f'_C(v)=\sum\limits_{j=1}^{n} c_j\beta(v;L_{S(n)}(v,j))$, where $c_k>0$ for $1\leq k\leq\rho(S(n))$. β is defined via Equation (18). We get,

$$f(v)=\begin{cases}c_1(\dfrac{1}{n-1}), & \text{if } v \text{ is the central vertex,}\\ c_1+c_2(\dfrac{1}{2n-3}), & \text{otherwise.}\end{cases} \tag{25}$$

Therefore,

$$\sum_{v\in V(S(n))} f(v)=c_1\left(\frac{1+(n-1)^2}{n-1}\right)+c_2\left(\frac{n-1}{2n-3}\right). \tag{26}$$

Thus,

$$p_f(v)=\begin{cases}\dfrac{c_1}{c_1(1+(n-1)^2)+c_2(\frac{(n-1)^2}{2n-3})}, & \text{if } v \text{ is the central vertex,}\\ \dfrac{c_1+c_2(\frac{1}{2n-3})}{c_1(\frac{1+(n-1)^2}{n-1})+c_2(\frac{n-1}{2n-3})}, & \text{otherwise.}\end{cases} \tag{27}$$

By substituting the value of $p_f(v)$ in $I_f(S(n))$ and simplifying, we get

$$I_f(S(n))=-x\log_2 x-(1-x)\log_2\left(\frac{1-x}{n-1}\right), \tag{28}$$

where $x=\dfrac{c_1}{c_1(1+(n-1)^2)+c_2(\dfrac{(n-1)^2}{2n-3})}$.

By choosing particular values for the parameters involved, we get concrete measures using the above stated functionals. For example, consider the functional $f=f_{P'}$ and set

$$c_1:=\rho(S(n))=2 \text{ and } c_2:=\rho(S(n))-1=1. \tag{29}$$

If we plug in those values in Equations (10) and (11), we easily derive

$$I_{f_{P'}}(S(n))=\frac{2}{n+2}\log_2\left(\frac{n+2}{2}\right)+\frac{n}{n+2}\log_2\left(\frac{(n+2)(n-1)}{n}\right). \tag{30}$$

Paths. Let P_n be the path graph on n vertices. Path graphs are the only trees with maximum diameter among all the trees on n vertices, i.e., $\rho(P_n)=n-1$. We remark that to compute a closed form expression even for path graphs, is not always simple. To illustrate this, we present the concrete information measure $I_{f_{P'}}(P_n)$ by choosing particular values for its coefficients.

Lemma 5 *Let P_n be a path graph and consider the functional $f=f_{P'}$ defined by Equation (6). We set $c_1:=\rho(P_n)=n-1$, $c_2:=\rho(P_n)-1,\ldots,c_\rho:=1$. We yield*

$$I_{f_{P'}}(P_n)=3\sum_{r=1}^{\lceil n/2\rceil}\left(\frac{n^2+n(2r-3)-2r(r-1)}{n(n-1)(2n-1)}\right)\log_2\left(\frac{2n(n-1)(2n-1)}{3n^2+3n(2r-3)-6r(r-1)}\right). \tag{31}$$

Proof: Let P_n be a path graph trivially labeled by $v_1, v_2,\ldots,v_n$ (from left to right).

Given $f(v)=f_{P'}(v)=\sum_{j=1}^{n-1} c_j|S_j(v;P_n)|$ with $c_j=n-j$ for $1\leq j\leq n-1$.

By computing f, when $v\in\{v_r,v_{n+1-r}\}$, for $1\leq r\leq\lceil\frac{n}{2}\rceil$, we infer

$$f(v)=\sum_{j=1}^{r-1}2c_j+\sum_{j=r}^{n-r}c_j, \tag{32}$$

$$=2\sum_{j=1}^{r-1}(n-j)+\sum_{j=r}^{n-r}(n-j), \quad (33)$$

$$=\frac{1}{2}[n^2+n(2r-3)-2r(r-1)]. \quad (34)$$

Therefore,

$$\sum_{i=1}^{n}f(v_i)=2\sum_{j=1}^{n-1}(n-j)c_j=\frac{1}{3}n(n-1)(2n-1), \quad (35)$$

and, hence,

$$p_f(v)=\frac{3}{2}\frac{n^2+n(2r-3)-2r(r-1)}{n(n-1)(2n-1)}, \quad (36)$$

where $v\in\{v_r,v_{n+1-r}\}$, for $1\leq r\leq\lceil\frac{n}{2}\rceil$. By substituting these quantities into $I_f(P_n)$ yields the desired result.

Note that when using the same measure with arbitrary coefficients, its computation is intricate. In this regard, we present explicit bounds or information inequalities for any connected graph if the measure is based on the information functional using j-spheres. That is, either $f=f_P$ or $f=f_{P'}$.

General connected graphs. **Theorem 6** *Given any connected graph $G=(V,E)$ on n vertices and let $f=f_P$ given by Equation (5). Then, we infer the following bounds:*

$$I_f(G)\leq\begin{cases}\alpha^X\log_2(n\cdot\alpha^X), & \text{if } \alpha>1,\\ \alpha^{-X}\log_2(n\cdot\alpha^{-X}), & \text{if } \alpha<1.\end{cases} \quad (37)$$

$$I_f(G)\geq\begin{cases}\alpha^X\log_2(n\cdot\alpha^X), & \text{if } \left(\frac{1}{n}\right)^{\frac{1}{X}}\leq\alpha\leq1,\\ \alpha^{-X}\log_2(n\cdot\alpha^{-X}), & \text{if } 1\leq\alpha\leq n^{\frac{1}{X}},\\ 0, & \text{if } 0<\alpha\leq\left(\frac{1}{n}\right)^{\frac{1}{X}} \text{ or } \alpha\geq n^{\frac{1}{X}}.\end{cases} \quad (38)$$

$$\text{where} \quad X=(c_{\max}-c_{\min})(n-1), \quad (38)$$

$$\text{with} \quad c_{\max}=\max\{c_j:1\leq j\leq\rho(G)\}, \quad (40)$$

$$\text{and} \quad c_{\min}=\min\{c_j:1\leq j\leq\rho(G)\}. \quad (41)$$

Proof: Consider $f(v)=f_P(v)=\alpha^{\sum_{j=1}^{\rho(G)}c_j|S_j(v;G)|}$, where $\alpha>0$ and $c_k>0$ for $1\leq k\leq\rho(G)$. Let $c_{\max}=\max\{c_j:1\leq j\leq\rho(G)\}$ and $c_{\min}=\min\{c_j:1\leq j\leq\rho(G)\}$. Recall (see Remark (2)) that, when either $\alpha=1$ or when all the coefficients (c_k) are equal, the information functional becomes constant and, hence, the value of $I_f(G)$ equals $\log_2 n$. In the following, we will discuss the cases $\alpha>1$ and $\alpha<1$, and we also assume that not all c_k are equal.

Case 1: $\alpha>1$: We first construct the bounds for $p_f(v)$ as shown below:

$$f(v)=\alpha^{\sum_{j=1}^{\rho(G)}c_j|S_j(v;G)|} \quad (42)$$

$$\leq\alpha^{(n-1)c_{\max}}. \quad (43)$$

Similarly,

$$f(v)\geq\alpha^{(n-1)c_{\min}}. \quad (44)$$

Therefore, from the Equations (43) and (44), we get

$$n\alpha^{(n-1)c_{\min}}\leq\sum_{v\in V}f(v)\leq n\alpha^{(n-1)c_{\max}}. \quad (45)$$

Hence,

$$\frac{\alpha^{(n-1)c_{\min}}}{n\cdot\alpha^{(n-1)c_{\max}}}\leq p_f(v)\leq\frac{\alpha^{(n-1)c_{\max}}}{n\cdot\alpha^{(n-1)c_{\min}}}. \quad (46)$$

Let $X=(n-1)[c_{\max}-c_{\min}]$. Then, the last inequality can be rewritten as,

$$\frac{1}{n\cdot\alpha^X}\leq p_f(v)\leq\frac{\alpha^X}{n}. \quad (47)$$

Upper bound for $I_f(G)$:

Since $X>0$ and $\alpha>1$, we have $\frac{1}{n\cdot\alpha^X}<1$. Hence, we have $-\log_2\frac{1}{n\cdot\alpha^X}\geq0$ and $0<-\log_2 p_f(v)\leq-\log_2\frac{1}{n\cdot\alpha^X}$. Thus we get,

$$-p_f(v)\log_2 p_f(v)\leq-\frac{\alpha^X}{n}\log_2\frac{1}{n\cdot\alpha^X}. \quad (48)$$

By adding over all the vertices of V, we obtain

$$I_f(G)\leq-\alpha^X\log_2\frac{1}{n\cdot\alpha^X}=\alpha^X\log_2(n\cdot\alpha^X). \quad (49)$$

Lower bound for $I_f(G)$:

We have to distinguish two cases, either $\alpha^X<n$ or $\alpha^X\geq n$.

Case 1.1: $1<\alpha<n^{1/X}$. We yield $-\log_2 p_f(v)\geq-\log_2\frac{\alpha^X}{n}>0$. Therefore,

$$-p_f(v)\log_2 p_f(v)\geq-\frac{1}{n\cdot\alpha^X}\log_2\frac{\alpha^X}{n}. \quad (50)$$

By adding over all the vertices of V, we get

$$I_f(G)\geq-\frac{1}{\alpha^X}\log_2\frac{\alpha^X}{n}=\alpha^{-X}\log_2(n\cdot\alpha^{-X}). \quad (51)$$

Case 1.2: $\alpha\geq n^{1/X}$.

In this case, we obtain $\log_2\frac{\alpha^X}{n}\geq0$ and $\log_2 p_f(v)<0\leq\log_2\frac{\alpha^X}{n}$. Therefore, by using these bounds in Equation (4), we infer $I_f(G)>0$.

Case 2: $\alpha<1$:

Consider Equation (42). We get the following bounds for $f(v)$:

$$\alpha^{(n-1)c_{\max}}\leq f(v)\leq\alpha^{(n-1)c_{\min}}. \quad (52)$$

Therefore,

$$n\alpha^{(n-1)c_{\max}} \leq \sum_{v\in V} f(v) \leq n\alpha^{(n-1)c_{\min}}. \tag{53}$$

Hence,

$$\frac{\alpha^{(n-1)c_{\max}}}{n\cdot\alpha^{(n-1)c_{\min}}} \leq p_f(v) \leq \frac{\alpha^{(n-1)c_{\min}}}{n\cdot\alpha^{(n-1)c_{\max}}}. \tag{54}$$

Set $X=(n-1)[c_{\max}-c_{\min}]$. Then, the last inequality can be rewritten as,

$$\frac{\alpha^X}{n} \leq p_f(v) \leq \frac{1}{n\cdot\alpha^X}. \tag{55}$$

Upper bound for $I_f(G)$:

Since $X>0$ and $\alpha<1$, we have $\frac{\alpha^X}{n}\leq 1$. Hence, we have $-\log_2\frac{\alpha^X}{n}\geq 0$ and $0<-\log_2 p_f(v)\leq -\log_2\frac{\alpha^X}{n}$. Thus, we obtain,

$$-p_f(v)\log_2 p_f(v) \leq -\frac{1}{n\cdot\alpha^X}\log_2\frac{\alpha^X}{n}. \tag{56}$$

By adding over all the vertices of V, we get

$$I_f(G) \leq -\frac{1}{\alpha^X}\log_2\frac{\alpha^X}{n} = \alpha^{-X}\log_2(n\cdot\alpha^{-X}). \tag{57}$$

Lower bound for $I_f(G)$:

Again, we consider two cases, either $\alpha^X\leq\frac{1}{n}$ or $\alpha^X>\frac{1}{n}$.

Case 2.1: $0<\alpha\leq(\frac{1}{n})^{1/X}$.

In this case, we have $\log_2\frac{1}{n\cdot\alpha^X}\geq 0$ and $\log_2 p_f(v)<0\leq\log_2\frac{1}{n\cdot\alpha^X}$. Therefore, by substituting these bounds in the Equation (4), we obtain $I_f(G)>0$.

Case 2.2: $(\frac{1}{n})^{1/X}<\alpha<1$.

We have $-\log_2 p_f(v)\geq-\log_2\frac{1}{n\alpha^X}>0$. Therefore,

$$-p_f(v)\log_2 p_f(v) \geq -\frac{\alpha^X}{n}\log_2\frac{1}{n\cdot\alpha^X}. \tag{58}$$

By adding over all the vertices of V, we get

$$I_f(G) \geq -\alpha^X\log_2\frac{1}{n\cdot\alpha^X} = \alpha^X\log_2(n\cdot\alpha^X). \tag{59}$$

Hence, the theorem follows.

In the next theorem, we obtain explicit bounds when using the information functional given by Equation (6).

Theorem 7 *Given any connected graph $G=(V,E)$ on n vertices and let $f=f'_P$ be given as in Equation (6). We yield*

$$I_f(G) \leq \frac{c_{\max}}{c_{\min}}\log_2\left(\frac{n\cdot c_{\max}}{c_{\min}}\right), \tag{60}$$

$$I_f(G) \geq \begin{cases} 0, & \text{if } n\leq\frac{c_{\max}}{c_{\min}}, \\ \frac{c_{\min}}{c_{\max}}\log_2\left(\frac{n\cdot c_{\min}}{c_{\max}}\right), & \text{if } n>\frac{c_{\max}}{c_{\min}}, \end{cases} \tag{61}$$

$$\text{with } c_{\max}=\max\{c_j : 1\leq j\leq\rho(G)\}, \tag{62}$$

$$\text{and } c_{\min}=\min\{c_j : 1\leq j\leq\rho(G)\}. \tag{63}$$

Proof: Consider $f(v)=f'_P(v)=\sum_{j=1}^{\rho(G)} c_j|S_j(v;G)|$, where $c_k>0$ for $1\leq k\leq\rho(G)$. Let $c_{\max}=\max\{c_j : 1\leq j\leq\rho(G)\}$ and $c_{\min}=\min\{c_j : 1\leq j\leq\rho(G)\}$. We have,

$$f(v)=\sum_{j=1}^{\rho(G)} c_j|S_j(v;G)| \leq (n-1)c_{\max}. \tag{64}$$

Similarly,

$$f(v)\geq(n-1)c_{\min}. \tag{65}$$

Therefore, from the Equations (64) and (65), we get

$$n(n-1)c_{\min} \leq \sum_{v\in V} f(v) \leq n(n-1)c_{\max}. \tag{66}$$

Hence,

$$\frac{c_{\min}}{n\cdot c_{\max}} \leq p_f(v) \leq \frac{c_{\max}}{n\cdot c_{\min}}. \tag{67}$$

Upper bound for $I_f(G)$:

Since $\frac{c_{\min}}{n\cdot c_{\max}}\leq 1$, we have $-\log_2\frac{c_{\min}}{n\cdot c_{\max}}\geq 0$ and $0<-\log_2 p_f(v)\leq-\log_2\frac{c_{\min}}{n\cdot c_{\max}}$. Hence,

$$-p_f(v)\log_2 p_f(v) \leq -\frac{c_{\max}}{n\cdot c_{\min}}\log_2\frac{c_{\min}}{n\cdot c_{\max}}. \tag{68}$$

By adding over all the vertices of V, we obtain

$$I_f(G) \leq -\frac{c_{\max}}{c_{\min}}\log_2\frac{c_{\min}}{n\cdot c_{\max}} = \frac{c_{\max}}{c_{\min}}\log_2\frac{n\cdot c_{\max}}{c_{\min}}. \tag{69}$$

Lower bound for $I_f(G)$:

Let us distinguish two cases:

Case 1: $c_{\max}\geq n\cdot c_{\min}$.

We have $\log_2\frac{c_{\max}}{n\cdot c_{\min}}\geq 0$ and $\log_2 p_f(v)<0\leq\log_2\frac{c_{\max}}{n\cdot c_{\min}}$. Therefore, by applying these bounds to Equation (4), we obtain $I_f(G)>0$.

Case 2: $c_{\max}<n\cdot c_{\min}$.

In this case, we have $-\log_2 p_f(v)\geq-\log_2\frac{c_{\max}}{n\cdot c_{\min}}>0$. Therefore,

$$-p_f(v)\log_2 p_f(v) \geq -\frac{c_{\min}}{n\cdot c_{\max}}\log_2\frac{c_{\max}}{n\cdot c_{\min}}. \tag{70}$$

By adding over all the vertices of V, we obtain the lower bound for $I_f(G)$ given by

$$I_f(G) \geq -\frac{c_{\min}}{c_{\max}}\log_2\frac{c_{\max}}{n\cdot c_{\min}} = \frac{c_{\min}}{c_{\max}}\log_2\frac{n\cdot c_{\min}}{c_{\max}}. \quad (71)$$

Hence, the theorem follows.

Implicit Information Inequalities

Information inequalities describe relations between information measures for graphs. An implicit information inequality is a special type of an information inequality where the entropy of the graph is estimated by a quantity that contains another graph entropy expression. In this section, we will present some implicit information inequalities for entropy measures based on information functionals. In this direction, a first attempt has been done by Dehmer et al. [23,24,26]. Note that Dehmer et al. [23,26] started from certain conditions on the probabilities when two different information functionals f and f^* are given. In contrast, we start from certain assumptions which the functionals themselves should satisfy and, finally, derive novel implicit inequalities. Now, given any graph $G=(V,E), |V|=n$. Let $I_{f_1}(G)$ and $I_{f_2}(G)$ be two mean information measures of G defined using the information functionals f_1 and f_2 respectively. Let us further define another functional $f(v)=c_1f_1(v)+c_2f_2(v),\ v\in V$. In the following, we will study the relation between the information measure $I_f(G)$ and the measures $I_{f_1}(G)$ and $I_{f_2}(G)$.

Theorem 8 *Suppose $f_1(v)\leq f_2(v)$, for all $v\in V$, then the information measure $I_f(G)$ can be bounded by $I_{f_1}(G)$ and $I_{f_2}(G)$ as follows:*

$$I_f(G) \geq \frac{(c_1+c_2)A_1}{A}\left(I_{f_1}(G) - \log_2\frac{c_1A_1}{A}\right) - \frac{c_2(c_1+c_2)A_2}{c_1A\ln(2)}, \quad (72)$$

$$I_f(G) \leq \frac{(c_1+c_2)A_2}{A}\left(I_{f_2}(G) - \log_2\frac{c_2A_2}{A}\right), \quad (73)$$

where $A=c_1A_1+c_2A_2$, $A_1=\sum_{v\in V} f_1(v)$, *and* $A_2=\sum_{v\in V} f_2(v)$.

Proof: Given $f(v)=c_1f_1(v)+c_2f_2(v)$. Let $A_1=\sum_{v\in V}f_1(v)$ and $A_2=\sum_{v\in V}f_2(v)$. Therefore $\sum_{v\in V}f(v)=c_1A_1+c_2A_2=:A$. The information measures of G with respect to f_1 and f_2 are given by

$$I_{f_1}(G) = -\sum_{v\in V} p_{f_1}(v)\log_2 p_{f_1}(v), \quad (74)$$

where $p_{f_1}(v)=\frac{f_1(v)}{\sum_{v\in V}f_1(v)}=\frac{f_1(v)}{A_1}$,

$$I_{f_2}(G) = -\sum_{v\in V} p_{f_2}(v)\log_2 p_{f_2}(v), \quad (75)$$

where $p_{f_2}(v)=\frac{f_2(v)}{\sum_{v\in V}f_2(v)}=\frac{f_2(v)}{A_2}$.

Now consider the probabilities,

$$p_f(v) = \frac{f(v)}{\sum_{v\in V}f(v)} = \frac{c_1f_1(v)+c_2f_2(v)}{A}, \quad (76)$$

$$= \frac{c_1A_1\cdot p_{f_1}(v)+c_2A_2\cdot p_{f_2}(v)}{A}, \quad (77)$$

$$\leq \frac{(c_1+c_2)A_2\cdot p_{f_2}(v)}{A}, \text{since } A_1\cdot p_{f_1}(v)\leq A_2\cdot p_{f_2}(v). \quad (78)$$

Using Equation (77) and based on the fact that $p_f(v)\leq 1$, we get

$$-\log_2 p_f(v) = -\log_2\left(\frac{c_1A_1\cdot p_{f_1}(v)+c_2A_2\cdot p_{f_2}(v)}{A}\right) \geq 0. \quad (79)$$

Thus,

$$-p_f(v)\log_2 p_f(v) \leq -\left(\frac{(c_1+c_2)A_2\cdot p_{f_2}(v)}{A}\right) \log_2\left(\frac{c_1A_1\cdot p_{f_1}(v)+c_2A_2\cdot p_{f_2}(v)}{A}\right), \quad (80)$$

and

$$-p_f(v)\log_2 p_f(v) \leq \left[\frac{(c_1+c_2)A_2}{A}\right]\left[-p_{f_2}(v)\log_2 p_{f_2}(v) - p_{f_2}(v)\log_2\frac{c_2A_2}{A}\right] - \left(\frac{(c_1+c_2)A_2p_{f_2}(v)}{A}\right)\log_2\left(1+\frac{c_1A_1p_{f_1}(v)}{c_2A_2p_{f_2}(v)}\right). \quad (81)$$

Since the last term in the above inequality is positive, we get

$$-p_f(v)\log_2 p_f(v) \leq \left[\frac{(c_1+c_2)A_2}{A}\right]\left[-p_{f_2}(v)\log_2 p_{f_2}(v) - p_{f_2}(v)\log_2\frac{c_2A_2}{A}\right]. \quad (82)$$

By adding up the above inequalities over all the vertices of V, we get the desired upper bound. From Equation (77), we also get a lower bound for $p_f(v)$, given by

$$p_f(v) \geq \frac{(c_1+c_2)A_1\cdot p_{f_1}(v)}{A}, \text{since } A_1\cdot p_{f_1}(v)\leq A_2\cdot p_{f_2}(v). \quad (83)$$

Now proceeding as before with the above inequality for $p_f(v)$, we obtain

$$-p_f(v)\log_2 p_f(v) \geq -\left(\frac{(c_1+c_2)A_1\cdot p_{f_1}(v)}{A}\right) \log_2\left(\frac{c_1A_1\cdot p_{f_1}(v)+c_2A_2\cdot p_{f_2}(v)}{A}\right). \quad (84)$$

$$-p_f(v)\log_2 p_f(v) \geq \left[\frac{(c_1+c_2)A_1}{A}\right]\left[-p_{f_1}(v)\log_2 p_{f_1}(v) - p_{f_1}(v)\log_2\frac{c_1A_1}{A}\right] - \left(\frac{(c_1+c_2)A_1p_{f_1}(v)}{A}\right)\log_2\left(1+\frac{c_2A_2p_{f_2}(v)}{c_1A_1p_{f_1}(v)}\right). \quad (85)$$

By using the concavity property of the logarithm, that is, $\log_2(1+\frac{x}{y}) \leq \frac{1}{\ln(2)}(\frac{x}{y})$, we yield

$$-p_f(v)\log_2 p_f(v) \geq \left[\frac{(c_1+c_2)A_1}{A}\right] \left[-p_{f_1}(v)\log_2 p_{f_1}(v) - p_{f_1}(v)\log_2\frac{c_1A_1}{A}\right] - \frac{(c_1+c_2)}{A}\cdot\frac{c_2A_2p_{f_2}(v)}{c_1\ln(2)}. \quad (86)$$

By adding the above inequality over all the vertices of V, we get the desired lower bound. This proves the theorem.

Corollary 9 *The information measure $I_f(G)$, for $f=f_1+f_2$, is bounded by $I_{f_1}(G)$ and $I_{f_2}(G)$ as follows:*

$$I_f(G) \geq \frac{2A_1}{A_1+A_2}\left(I_{f_1}(G) - \log_2\frac{A_1}{A_1+A_2}\right) - \frac{2A_2\log_2 e}{(A_1+A_2)}, \quad (87)$$

$$I_f(G) \leq \frac{2A_2}{A_1+A_2}\left(I_{f_2}(G) - \log_2\frac{A_2}{A_1+A_2}\right). \quad (88)$$

Proof: Set $c_1=c_2$ in Theorem (8), then the corollary follows.

Corollary 10 *Given two information functionals, f_1, f_2 such that $f_1(v) \leq f_2(v)$, $\forall v \in V$. Then*

$$I_{f_1}(G) \leq \frac{A_2}{A_1}I_{f_2}(G) + \log_2\frac{A_1}{A_1+A_2} - \frac{A_2}{A_1}\log_2\frac{A_2}{A_1+A_2} + \frac{A_2\log_2 e}{A_1}. \quad (89)$$

Proof: Follows from Corollary (9).

The next theorem gives another bound for I_f in terms of both I_{f_1} and I_{f_2} by using the concavity property of the logarithmic function.

Theorem 11 *Let $f_1(v)$ and $f_2(v)$ be two arbitrary functionals defined on a graph G. If $f(v)=c_1f_1(v)+c_2f_2(v)$ for all $v\in V$, we infer*

$$I_f(G) \geq \frac{c_1A_1}{A}\left[I_{f_1}(G) - \log_2\frac{c_1A_1}{A}\right] + \frac{c_2A_2}{A}\left[I_{f_2}(G) - \log_2\frac{c_2A_2}{A}\right] - \log_2 e. \quad (90)$$

and

$$I_f(G) \leq \frac{c_1A_1}{A}\left[I_{f_1}(G) - \log_2\frac{c_1A_1}{A}\right] + \frac{c_2A_2}{A}\left[I_{f_2}(G) - \log_2\frac{c_2A_2}{A}\right], \quad (91)$$

where $A=c_1A_1+c_2A_2$, $A_1=\sum_{v\in V} f_1(v)$ and $A_2=\sum_{v\in V} f_2(v)$.

Proof: Starting from the quantities for $p_f(v)$ based on Equation (77), we obtain

$$p_f(v)\log_2 p_f(v) = \left(\frac{c_1A_1\cdot p_{f_1}(v)+c_2A_2\cdot p_{f_2}(v)}{A}\right) \log_2\left(\frac{c_1A_1\cdot p_{f_1}(v)+c_2A_2\cdot p_{f_2}(v)}{A}\right), \quad (92)$$

$$= \frac{c_1A_1\cdot p_{f_1}(v)}{A}\log_2\left[\left(\frac{c_1A_1\cdot p_{f_1}(v)}{A}\right)\left(1+\frac{c_2A_2\cdot p_{f_2}(v)}{c_1A_1\cdot p_{f_1}(v)}\right)\right] + \frac{c_2A_2\cdot p_{f_2}(v)}{A}\log_2\left[\left(\frac{c_2A_2\cdot p_{f_2}(v)}{A}\right)\left(1+\frac{c_1A_1\cdot p_{f_1}(v)}{c_2A_2\cdot p_{f_2}(v)}\right)\right], \quad (93)$$

$$= \frac{c_1A_1\cdot p_{f_1}(v)}{A}\left\{\log_2\left(\frac{c_1A_1\cdot p_{f_1}(v)}{A}\right) + \log_2\left(1+\frac{c_2A_2\cdot p_{f_2}(v)}{c_1A_1\cdot p_{f_1}(v)}\right)\right\} + \frac{c_2A_2\cdot p_{f_2}(v)}{A}\left\{\log_2\left(\frac{c_2A_2\cdot p_{f_2}(v)}{A}\right) + \log_2\left(1+\frac{c_1A_1\cdot p_{f_1}(v)}{c_2A_2\cdot p_{f_2}(v)}\right)\right\}, \quad (94)$$

$$= \frac{c_1A_1}{A}\left\{p_{f_1}(v)\log_2 p_{f_1}(v) + p_{f_1}(v)\log_2\frac{c_1A_1}{A}\right\} + \frac{c_2A_2}{A}\left\{p_{f_2}(v)\log_2 p_{f_2}(v) + p_{f_2}(v)\log_2\frac{c_2A_2}{A}\right\} + \frac{c_1A_1p_{f_1}(v)}{A}\log_2\left(1+\frac{c_2A_2\cdot p_{f_2}(v)}{c_1A_1\cdot p_{f_1}(v)}\right) + \frac{c_2A_2p_{f_2}(v)}{A}\log_2\left(1+\frac{c_1A_1\cdot p_{f_1}(v)}{c_2A_2\cdot p_{f_2}(v)}\right). \quad (95)$$

Since each of the last two terms in Equation (95) is positive, we get a lower bound for $p_f(v)\log_2 p_f(v)$, given by

$$p_f(v)\log_2 p_f(v) \geq \frac{c_1A_1}{A}\left\{p_{f_1}(v)\log_2 p_{f_1}(v) + p_{f_1}(v)\log_2\frac{c_1A_1}{A}\right\} + \frac{c_2A_2}{A}\left\{p_{f_2}(v)\log_2 p_{f_2}(v) + p_{f_2}(v)\log_2\frac{c_2A_2}{A}\right\}. \quad (96)$$

Applying the last inequality to Equation (4), we get the upper bound as given in Equation (91). By further applying the inequality $\log_2(1+\frac{x}{y}) \leq \frac{1}{\ln(2)}(\frac{x}{y})$ to Equation (95), we get an upper bound for $p_f(v)\log_2 p_f(v)$, given by

$$p_f(v)\quad\log_2 p_f(v) \leq \frac{c_1A_1}{A}\left\{p_{f_1}(v)\log_2 p_{f_1}(v) + p_{f_1}(v)\log_2\frac{c_1A_1}{A}\right\} + \frac{c_2A_2}{A}\left\{p_{f_2}(v)\log_2 p_{f_2}(v) + p_{f_2}(v)\log_2\frac{c_2A_2}{A}\right\} + \frac{c_1A_1p_{f_1}(v)}{A\ln(2)}\left(\frac{c_2A_2p_{f_2}(v)}{c_1A_1p_{f_1}(v)}\right) + \frac{c_2A_2p_{f_2}(v)}{A\ln(2)}\left(\frac{c_1A_1\cdot p_{f_1}(v)}{c_2A_2\cdot p_{f_2}(v)}\right). \quad (97)$$

Therefore,

$$p_f(v)\log_2 p_f(v) \leq \frac{c_1A_1}{A}\left\{p_{f_1}(v)\log_2 p_{f_1}(v) + p_{f_1}(v)\log_2\frac{c_1A_1}{A}\right\} + \frac{c_2A_2}{A}\left\{p_{f_2}(v)\log_2 p_{f_2}(v) + p_{f_2}(v)\log_2\frac{c_2A_2}{A}\right\} + \frac{1}{\ln(2)}\cdot\frac{c_1A_1p_{f_1}(v)+c_2A_2p_{f_2}(v)}{A}. \quad (98)$$

Finally, we now apply this inequality to Equation (4) and get the lower bound as given in Equation (90).

The next theorem is a straightforward extension of the previous statement. Here, an information functional is expressed as a linear combination of k arbitrary information functionals.

Theorem 12 *Let $k \geq 2$ and $f_1(v), f_2(v), \ldots, f_k(v)$ be arbitrary functionals defined on a graph G. $I_{f_1}(G), I_{f_2}(G), \ldots, I_{f_k}(G)$ are the corresponding information contents. If $f(v) = c_1 f_1(v) + c_2 f_2(v) + \cdots + c_k f_k(v)$ for all $v \in V$, we infer*

$$I_f(G) \geq \sum_{i=1}^{k} \left\{ \frac{c_i A_i}{A} \left[I_{f_i}(G) - \log_2 \frac{c_i A_i}{A} \right] \right\} - (k-1) \log_2 e, \quad (99)$$

and

$$I_f(G) \leq \sum_{i=1}^{k} \left\{ \frac{c_i A_i}{A} \left[I_{f_i}(G) - \log_2 \frac{c_i A_i}{A} \right] \right\}, \quad (100)$$

where $A = \sum_{i=1}^{k} c_i A_i$, $A_j = \sum_{v \in V} f_j(v)$ for $1 \leq j \leq k$.

Union of Graphs. In this section, we determine the entropy of the union of two graphs. Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two arbitrary connected graphs on n_1 and n_2 vertices, respectively. Let f be an information functional defined on these graphs denoted by f_{G_1}, f_{G_2} and let $I_f(G_1)$ and $I_f(G_2)$ be the information measures on G_1 and G_2 respectively.

Theorem 13 *Let $G = (V, E) = G_1 \cup G_2$ be the disjoint union of the graphs G_1 and G_2. Let f be an arbitrary information functional. The information measure $I_f(G)$ can be expressed in terms of $I_f(G_1)$ and $I_f(G_2)$ as follows:*

$$I_f(G) = \frac{A_1}{A}\left(I_f(G_1) - \log_2 \frac{A_1}{A} \right) + \frac{A_2}{A}\left(I_f(G_2) - \log_2 \frac{A_2}{A} \right), \quad (101)$$

where $A = A_1 + A_2$ with $A_1 = \sum_{v \in V_1} f_{G_1}(v)$ and $A_2 = \sum_{v \in V_2} f_{G_2}(v)$.

Proof: Let f be the given information functional. Let $A_1 = \sum_{v \in V_1} f_{G_1}(v)$ and $A_2 = \sum_{v \in V_2} f_{G_2}(v)$. The information measures of G_1 and G_2 are given as follows:

$$I_f(G_1) = -\sum_{v \in V_1} p_{G_1}(v) \log_2 p_{G_1}(v), \quad (102)$$

where $p_{G_1}(v) = \frac{f_{G_1}(v)}{A_1}$, and

$$I_f(G_2) = -\sum_{v \in V_2} p_{G_2}(v) \log_2 p_{G_2}(v), \quad (103)$$

where $p_{G_2}(v) = \frac{f_{G_2}(v)}{A_2}$. For $v \in V$,

$$f(v) = \begin{cases} f_{G_1}(v), & \text{if } v \in V_1, \\ f_{G_2}(v), & \text{if } v \in V_2. \end{cases} \quad (104)$$

Hence,

$$\sum_{v \in V} f(v) = \sum_{v \in V_1} f(v) + \sum_{v \in V_2} f(v) = A_1 + A_2 =: A. \quad (105)$$

$$p_G(v) = \frac{f(v)}{\sum_{v \in V} f(v)} = \begin{cases} \frac{f_{G_1}(v)}{A}, & \text{if } v \in V_1, \\ \frac{f_{G_2}(v)}{A}, & \text{if } v \in V_2. \end{cases} \quad (106)$$

$$= \begin{cases} \frac{A_1}{A} \cdot p_{G_1}(v), & \text{if } v \in V_1, \\ \frac{A_2}{A} \cdot p_{G_2}(v), & \text{if } v \in V_2. \end{cases} \quad (107)$$

Using these quantities to determine $I_f(G)$, we obtain

$$\begin{aligned} I_f(G) &= -\sum_{v \in V_1} \frac{A_1 \cdot p_{G_1}(v)}{A} \log_2 \left(\frac{A_1 \cdot p_{G_1}(v)}{A} \right) \\ &\quad - \sum_{v \in V_2} \frac{A_2 \cdot p_{G_2}(v)}{A} \log_2 \left(\frac{A_2 \cdot p_{G_2}(v)}{A} \right), \end{aligned} \quad (108)$$

and

$$\begin{aligned} I_f(G) = &-\frac{A_1}{A} \sum_{v \in V_1} \left(p_{G_1}(v) \log_2 p_{G_1}(v) + p_{G_1}(v) \log_2 \left(\frac{A_1}{A}\right) \right) \\ &- \frac{A_2}{A} \sum_{v \in V_2} \left(p_{G_2}(v) \log_2 p_{G_2}(v) + p_{G_2}(v) \log_2 \left(\frac{A_2}{A}\right) \right). \end{aligned} \quad (109)$$

Upon simplification, we get the desired result.

Also, we immediately obtain a generalization of the previous theorem by taking k-disjoint graphs into account.

Theorem 14 *Let $G_1 = (V_1, E_1)$, $G_2 = (V_2, E_2), \ldots, G_k = (V_k, E_k)$ be k arbitrary connected graphs on $n_1, n_2, \ldots, n_k$ vertices, respectively. Let f be an information functional defined on these graphs denoted by $f_{G_1}, f_{G_2}, \ldots, f_{G_k}$. Let $G = (V, E) = G_1 \cup G_2 \cup \cdots \cup G_k$ be the disjoint union of the graphs $G_1, G_2, \ldots, G_k$ for $k \geq 2$. The information measure $I_f(G)$ can be expressed in terms of $I_f(G_1), I_f(G_2), \ldots, I_f(G_k)$ as follows:*

$$I_f(G) = \sum_{i=1}^{k} \left\{ \frac{A_i}{A} \left(I_f(G_i) - \log_2 \frac{A_i}{A} \right) \right\}, \quad (110)$$

where $A = A_1 + A_2 + \cdots + A_k$ with $A_i = \sum_{v \in V_1} f_{G_i}(v)$ for $1 \leq i \leq k$.

Join of Graphs. Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two arbitrary connected graphs on n_1 and n_2 vertices, respectively. The join of the graphs $G_1 + G_2$ is defined as the graph $G = (V, E)$ with vertex set $V = V_1 \cup V_2$ and the edge set $E = E_1 \cup E_2 \cup \{(x, y) : x \in V_1, y \in V_2\}$. Let $f = f_P$ be the information functional (given by Equation (5)) based on the j-sphere functional (exponential) defined on these graphs and denoted by f_{G_1}, f_{G_2}. Let $I_f(G_1)$ and $I_f(G_2)$ be the information measures on G_1 and G_2 respectively.

Theorem 15 *Let $G = (V, E) = G_1 + G_2$ be the join of the graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ with $n_1 + n_2$ vertices. The information measure $I_f(G)$ can then be expressed in terms of $I_f(G_1)$ and $I_f(G_2)$ as follows:*

$$I_f(G) = \frac{A_1\alpha^{c_1 n_2}}{A}\left(I_f(G_1) - \log_2\frac{A_1\alpha^{c_1 n_2}}{A}\right) + \frac{A_2\alpha^{c_1 n_1}}{A}\left(I_f(G_2) - \log_2\frac{A_2\alpha^{c_1 n_2}}{A}\right), \quad (111)$$

where $f_H(v) = \alpha^{\sum_{j=1}^{\rho(H)} c_j S_j(v;H)}$ *for* $H \in \{G_1, G_2, G\}$, $c_j > 0$ *and* $A = A_1\alpha^{c_1 n_2} + A_2\alpha^{c_1 n_1}$ *with* $A_1 = \sum_{v\in V_1} f_{G_1}(v)$ *and* $A_2 = \sum_{v\in V_2} f_{G_2}(v)$.

Proof: Let $G = G_1 + G_2$ be the join of two connected graphs G_1 and G_2. Here, $\rho(G) = \max\{\rho(G_1), \rho(G_2)\}$. Let $f_H(v) = \alpha^{\sum_{j=1}^{\rho(H)} c_j S_j(v;H)}$ be the information functional defined by using the j-sphere functional on $H \in \{G, G_1, G_2\}$. Let $A_1 = \sum_{v\in V_1} f_{G_1}(v)$ and $A_2 = \sum_{v\in V_2} f_{G_2}(v)$. The information measures of G_1 and G_2 are given as follows:

$$I_f(G_1) = -\sum_{v\in V_1} p_{G_1}(v)\log_2 p_{G_1}(v), \quad (112)$$

where $p_{G_1}(v) = \frac{f_{G_1}(v)}{A_1}$, and

$$I_f(G_2) = -\sum_{v\in V_2} p_{G_2}(v)\log_2 p_{G_2}(v), \quad (113)$$

where $p_{G_2}(v) = \frac{f_{G_2}(v)}{A_2}$. For $v \in V$,

$$f(v) = \begin{cases} \alpha^{c_1 n_2 + \sum_{j=1}^{\rho(G_1)} c_j S_j(v;G_1)}, & \text{if } v \in V_1, \\ \alpha^{c_1 n_1 + \sum_{j=1}^{\rho(G_2)} c_j S_j(v;G_2)}, & \text{if } v \in V_2. \end{cases} \quad (114)$$

$$= \begin{cases} \alpha^{c_1 n_2} f_{G_1}(v), & \text{if } v \in V_1, \\ \alpha^{c_1 n_1} f_{G_2}(v), & \text{if } v \in V_2. \end{cases} \quad (115)$$

Hence,

$$\sum_{v\in V} f(v) = \sum_{v\in V_1} f(v) + \sum_{v\in V_2} f(v) = A_1\alpha^{c_1 n_2} + A_2\alpha^{c_1 n_1} =: A, \quad (116)$$

$$p_G(v) = \frac{f_G(v)}{\sum_{v\in V} f(v)} = \begin{cases} \frac{\alpha^{c_1 n_2} f_{G_1}(v)}{A}, & \text{if } v \in V_1, \\ \frac{\alpha^{c_1 n_1} f_{G_2}(v)}{A}, & \text{if } v \in V_2. \end{cases} \quad (117)$$

$$= \begin{cases} \frac{\alpha^{c_1 n_2} A_1}{A} \cdot p_{G_1}(v), & \text{if } v \in V_1, \\ \frac{\alpha^{c_1 n_1} A_2}{A} \cdot p_{G_2}(v), & \text{if } v \in V_2. \end{cases} \quad (118)$$

Using those entities to determine $I_f(G)$, we infer

$$\begin{aligned} I_f(G) &= -\sum_{v\in V_1} \frac{\alpha^{c_1 n_2} A_1 \cdot p_{G_1}(v)}{A} \log_2\left(\frac{\alpha^{c_1 n_2} A_1 \cdot p_{G_1}(v)}{A}\right) \\ &\quad - \sum_{v\in V_2} \frac{\alpha^{c_1 n_1} A_2 \cdot p_{G_2}(v)}{A} \log_2\left(\frac{\alpha^{c_1 n_1} A_2 \cdot p_{G_2}(v)}{A}\right), \end{aligned} \quad (119)$$

and

$$\begin{aligned} I_f(G) &= -\frac{\alpha^{c_1 n_2} A_1}{A} \sum_{v\in V_1} \left(p_{G_1}(v)\log_2 p_{G_1}(v) + p_{G_1}(v)\log_2\left(\frac{\alpha^{c_1 n_2} A_1}{A}\right)\right) \\ &\quad - \frac{\alpha^{c_1 n_1} A_2}{A} \sum_{v\in V_2} \left(p_{G_2}(v)\log_2 p_{G_2}(v) + p_{G_2}(v)\log_2\frac{\alpha^{c_1 n_1} A_2}{A}\right). \end{aligned} \quad (120)$$

Upon simplification, we get the desired result.

If we consider the linear j-sphere functional f'_P (see Equation (6)), to infer an exact expression for the join of two graphs as in Theorem (15) is an intricate problem. By Theorem (16) and Theorem (17), we will now present different bounds in terms of $I_{f'_P}(G_1)$ and $I_{f'_P}(G_2)$.

Theorem 16 *Let* $G = (V, E) = G_1 + G_2$ *be the join of the graphs* $G_1 = (V_1, E_1)$ *and* $G_2 = (V_2, E_2)$ *on* $n_1 + n_2$ *vertices. Then, we yield*

$$I_f(G) \geq \frac{A_1}{A}\left(I_f(G_1) - \log_2\frac{A_1}{A}\right) + \frac{A_2}{A}\left(I_f(G_2) - \log_2\frac{A_2}{A}\right) - \frac{2c_1 n_1 n_2}{A\ln(2)}, \quad (121)$$

where $f_H(v) = \sum_{j=1}^{\rho(H)} c_j S_j(v;H)$ *for* $H \in \{G_1, G_2, G\}$, $c_j > 0$ *and* $A = 2c_1 n_1 n_2 + A_1 + A_2$ *with* $A_1 = \sum_{v\in V_1} f_{G_1}(v)$ *and* $A_2 = \sum_{v\in V_2} f_{G_2}(v)$.

Proof: Let $A_1 = \sum_{v\in V_1} f_{G_1}(v)$ and $A_2 = \sum_{v\in V_2} f_{G_2}(v)$. The information measures of G_1 and G_2 are given as follows:

$$I_f(G_1) = -\sum_{v\in V_1} p_{G_1}(v)\log_2 p_{G_1}(v), \quad (122)$$

where $p_{G_1}(v) = \frac{f_{G_1}(v)}{A_1}$, and

$$I_f(G_2) = -\sum_{v\in V_2} p_{G_2}(v)\log_2 p_{G_2}(v), \quad (123)$$

where $p_{G_2}(v) = \frac{f_{G_2}(v)}{A_2}$. For $v \in V$,

$$f(v) = \begin{cases} c_1 n_2 + \sum_{j=1}^{\rho(G_1)} c_j S_j(v;G_1), & \text{if } v \in V_1, \\ c_1 n_1 + \sum_{j=1}^{\rho(G_2)} c_j S_j(v;G_2), & \text{if } v \in V_2. \end{cases} \quad (124)$$

$$= \begin{cases} c_1 n_2 + f_{G_1}(v), & \text{if } v \in V_1, \\ c_1 n_1 + f_{G_2}(v), & \text{if } v \in V_2. \end{cases} \quad (125)$$

Hence,

$$\sum_{v\in V} f_G(v) = \sum_{v\in V_1} f_G(v) + \sum_{v\in V_2} f_G(v) = 2c_1n_1n_2 + A_1 + A_2 =: A. \tag{126}$$

$$p_G(v) = \frac{f_G(v)}{\sum_{v\in V} f_G(v)} = \begin{cases} \dfrac{c_1n_2 + f_{G_1}(v)}{A}, & \text{if } v\in V_1,\\ \dfrac{c_1n_1 + f_{G_2}(v)}{A}, & \text{if } v\in V_2. \end{cases} \tag{127}$$

$$= \begin{cases} \dfrac{A_1\cdot p_{G_1}(v)}{A} + \dfrac{c_1n_2}{A}, & \text{if } v\in V_1,\\ \dfrac{A_2\cdot p_{G_2}(v)}{A} + \dfrac{c_1n_1}{A}, & \text{if } v\in V_2. \end{cases} \tag{128}$$

Since $\frac{c_1n_2}{A}$ and $\frac{c_1n_1}{A}$ are positive, we get a lower bound for $p_G(v)$ given as

$$p_G(v) \geq \begin{cases} \dfrac{p_{G_1}(v)\cdot A_1}{A}, & \text{if } v\in V_1,\\ \dfrac{p_{G_2}(v)\cdot A_2}{A}, & \text{if } v\in V_2. \end{cases} \tag{129}$$

To infer a lower bound for the information measure $I_f(G)$, we start from the Equations (128), (129) and obtain

$$-p_G(v)\log_2 p_G(v)$$
$$\geq \begin{cases} -\left(\dfrac{p_{G_1}(v)\cdot A_1}{A}\right)\log_2\left(\dfrac{p_{G_1}(v)A_1 + c_1n_2}{A}\right), & \text{if } v\in V_1,\\ -\left(\dfrac{p_{G_2}(v)\cdot A_2}{A}\right)\log_2\left(\dfrac{p_{G_2}(v)A_2 + c_1n_1}{A}\right), & \text{if } v\in V_2. \end{cases} \tag{130}$$

$$= \begin{cases} -\dfrac{A_1p_{G_1}(v)}{A}\log_2\left[\dfrac{A_1p_{G_1}(v)}{A}\left(1+\dfrac{c_1n_2}{A_1p_{G_1}(v)}\right)\right], & \text{if } v\in V_1,\\ -\dfrac{A_2p_{G_2}(v)}{A}\log_2\left[\dfrac{A_2p_{G_2}(v)}{A}\left(1+\dfrac{c_1n_1}{A_2p_{G_2}(v)}\right)\right], & \text{if } v\in V_2. \end{cases} \tag{131}$$

$$= \begin{cases} -\dfrac{A_1}{A}\left(p_{G_1}(v)\log_2 p_{G_1}(v) + p_{G_1}(v)\log_2\dfrac{A_1}{A}\right) \\ \qquad -\dfrac{A_1p_{G_1}(v)}{A}\log_2\left(1+\dfrac{c_1n_2}{A_1p_{G_1}(v)}\right), & \text{if } v\in V_1,\\ -\dfrac{A_2}{A}\left(p_{G_2}(v)\log_2 p_{G_2}(v) + p_{G_2}(v)\log_2\dfrac{A_2}{A}\right) \\ \qquad -\dfrac{A_2p_{G_2}(v)}{A}\log_2\left(1+\dfrac{c_1n_1}{A_2p_{G_2}(v)}\right), & \text{if } v\in V_2. \end{cases} \tag{132}$$

By using the inequality $\log_2\left(1+\frac{x}{y}\right) \leq \frac{1}{\ln(2)}\left(\frac{x}{y}\right)$ and performing simplification steps, we get,

$$-p_G(v)\log_2 p_G(v) \geq$$
$$\begin{cases} -\dfrac{A_1}{A}\left(p_{G_1}(v)\log_2 p_{G_1}(v) + p_{G_1}(v)\log_2\dfrac{A_1}{A}\right) - \dfrac{c_1n_2}{A\ln(2)}, \\ \qquad \text{if } v\in V_1,\\ -\dfrac{A_2}{A}\left(p_{G_2}(v)\log_2 p_{G_2}(v) + p_{G_2}(v)\log_2\dfrac{A_2}{A}\right) - \dfrac{c_1n_1}{A\ln(2)}, \\ \qquad \text{if } v\in V_2. \end{cases} \tag{133}$$

By adding up the above inequality system (across all the vertices of V) and by simplifying, we get the desired lower bound.

Further, an alternate set of bounds can be achieved as follows.

Theorem 17 *Let $G=(V,E)=G_1+G_2$ be the join of the graphs $G_1=(V_1,E_1)$ and $G_2=(V_2,E_2)$ on n_1+n_2 vertices. Then, we infer*

$$I_f(G) \leq \frac{A_1}{A}\left(I_f(G_1) - \log_2\frac{A_1}{A}\right) + \frac{A_2}{A}\left(I_f(G_2) - \log_2\frac{A_2}{A}\right) - \frac{c_1n_1n_2}{A}\log_2\frac{c_1^2n_1n_2}{A^2}, \tag{134}$$

and

$$I_f(G) \geq \frac{A_1}{A}\left(I_f(G_1) - \log_2\frac{A_1}{A}\right) + \frac{A_2}{A}\left(I_f(G_2) - \log_2\frac{A_2}{A}\right) - \frac{c_1n_1n_2}{A}\log_2\frac{c_1^2n_1n_2}{A^2} - \log_2(e), \tag{135}$$

where $f(v)=\sum_{j=1}^{\rho(H)} c_jS_j(v;H)$ for $H\in\{G_1,G_2,G\}$, $c_j>0$ and $A=2c_1n_1n_2+A_1+A_2$ with $A_1=\sum_{v\in V_1} f_{G_1}(v)$ and $A_2=\sum_{v\in V_2} f_{G_2}(v)$.

Proof: Starting from Theorem (16), consider the value of $p_G(v)$ given by Equation (128). By using the quantities for $p_G(v)$ to calculate $I_f(G)$, we get

$$I_f(G) = -\sum_{v\in V_1}\left(\frac{A_1\cdot p_{G_1}(v)+c_1n_2}{A}\right)\log_2\left(\frac{A_1\cdot p_{G_1}(v)+c_1n_2}{A}\right) - \sum_{v\in V_2}\left(\frac{A_2\cdot p_{G_2}(v)+c_1n_1}{A}\right)\log_2\left(\frac{A_2\cdot p_{G_2}(v)+c_1n_1}{A}\right), \tag{136}$$

and

$$\begin{aligned} I_f(G) = &-\frac{A_1}{A}\sum_{v\in V_1}\left(p_{G_1}(v)\log_2 p_{G_1}(v) + p_{G_1}(v)\log_2\frac{A_1}{A}\right) \\ &-\frac{A_1}{A}\sum_{v\in V_1} p_{G_1}(v)\log_2\left(1+\frac{c_1n_2}{A_1\cdot p_{G_1}(v)}\right) \\ &-\frac{c_1n_2}{A}\sum_{v\in V_1}\left(\log_2\frac{c_1n_2}{A} + \log_2\left(1+\frac{p_{G_1}(v)A_1}{c_1n_2}\right)\right) \\ &-\frac{A_2}{A}\sum_{v\in V_2} p_{G_2}(v)\left(\log_2 p_{G_2}(v) + \log_2\frac{A_2}{A}\right) \\ &-\frac{A_2}{A}\sum_{v\in V_2} p_{G_2}(v)\log_2\left(1+\frac{c_1n_1}{A_2\cdot p_{G_2}(v)}\right) \\ &-\frac{c_1n_1}{A}\sum_{v\in V_2}\left(\log_2\frac{c_1n_1}{A} + \log_2\left(1+\frac{p_{G_2}(v)A_2}{c_1n_1}\right)\right). \end{aligned} \tag{137}$$

By simplifying and performing summation, we get

$$\begin{aligned}I_f(G) = &\frac{A_1}{A}\left(I_f(G_1) - \log_2\frac{A_1}{A}\right) + \frac{A_2}{A}\left(I_f(G_2) - \log_2\frac{A_2}{A}\right)\\ &- \frac{c_1 n_1 n_2}{A}\log_2\frac{c_1^2 n_1 n_2}{A^2}\\ &- \frac{A_1}{A}\sum_{v\in V_1} p_{G_1}(v)\log_2\left(1+\frac{c_1 n_2}{A_1\cdot p_{G_1}(v)}\right)\\ &- \frac{c_1 n_2}{A}\sum_{v\in V_1}\log_2\left(1+\frac{p_{G_1}(v)A_1}{c_1 n_2}\right)\\ &- \frac{A_2}{A}\sum_{v\in V_2} p_{G_2}(v)\log_2\left(1+\frac{c_1 n_1}{A_2\cdot p_{G_2}(v)}\right)\\ &- \frac{c_1 n_1}{A}\sum_{v\in V_2}\log_2\left(1+\frac{p_{G_2}(v)A_2}{c_1 n_1}\right).\end{aligned} \tag{138}$$

An upper bound for the measure $I_f(G)$ can be derived as follows:

$$\begin{aligned}I_f(G) \le &\frac{A_1}{A}\left(I_f(G_1) - \log_2\frac{A_1}{A}\right) + \frac{A_2}{A}\left(I_f(G_2) - \log_2\frac{A_2}{A}\right)\\ &- \frac{c_1 n_1 n_2}{A}\log_2\frac{c_1^2 n_1 n_2}{A^2},\end{aligned} \tag{139}$$

since each of the remaining terms in Equation (138) is positive. Finally, we infer the lower bound for $I_f(G)$ as follows. By applying inequality $\log_2\left(1+\frac{x}{y}\right) \le \frac{1}{\ln(2)}\left(\frac{x}{y}\right)$ to Equation (138), we get

$$\begin{aligned}I_f(G) \ge &\frac{A_1}{A}\left(I_f(G_1) - \log_2\frac{A_1}{A}\right) + \frac{A_2}{A}\left(I_f(G_2) - \log_2\frac{A_2}{A}\right)\\ &- \frac{c_1 n_1 n_2}{A}\log_2\frac{c_1^2 n_1 n_2}{A^2} - \frac{A_1}{A}\sum_{v\in V_1} p_{G_1}(v)\left(\frac{c_1 n_2}{\ln(2)\cdot A_1\cdot p_{G_1}(v)}\right)\\ &- \frac{c_1 n_2}{A}\sum_{v\in V_1}\frac{p_{G_1}(v)A_1}{\ln(2)\cdot c_1 n_2} - \frac{A_2}{A}\sum_{v\in V_2} p_{G_2}(v)\left(\frac{c_1 n_1}{\ln(2)\cdot A_2\cdot p_{G_2}(v)}\right)\\ &- \frac{c_1 n_1}{A}\sum_{v\in V_2}\frac{p_{G_2}(v)A_2}{\ln(2)\cdot c_1 n_1}.\end{aligned} \tag{140}$$

Upon simplification, we get

$$\begin{aligned}I_f(G) \ge &\frac{A_1}{A}\left(I_f(G_1) - \log_2\frac{A_1}{A}\right) + \frac{A_2}{A}\left(I_f(G_2) - \log_2\frac{A_2}{A}\right)\\ &- \frac{c_1 n_1 n_2}{A}\log_2\frac{c_1^2 n_1 n_2}{A^2} - \frac{1}{\ln(2)}.\end{aligned} \tag{141}$$

Putting Inequality (139) and Inequality (141) together finishes the proof of the theorem.

Summary and Conclusion

In this article, we have investigated a challenging problem in quantitative graph theory namely to establish relations between graph entropy measures. Among the existing graph entropy measures, we have considered those entropies which are based on information functionals. It turned out that these measures have widely been applicable and useful when measuring the complexity of networks [3].

In general, to find relations between quantitative network measures is a daunting problem. The results could be used in various branches of science including mathematics, statistics, information theory, biology, chemistry and social sciences. Further, the determination of analytical relations between measures is of great practical importance when dealing with large scale networks. Also, relations involving quantitative network measures could be fruitful when determining the information content of large complex networks.

Note that our proof technique follows the one proposed in [23]. It is based on three main steps: Firstly, we compute the information functionals and in turn, we calculate the probability values for every vertex of the graph in question. Secondly, we start with certain conditions for the computed functionals and arrive at a system of inequalities. Thirdly, by adding up the corresponding inequality system, we obtain the desired implicit information inequality. Using this approach, we have inferred novel bounds by assuming certain information functionals. It is evident that further bounds could be inferred by taking novel information functionals into account. Further, we explored relations between the involved information measures for general connected graphs and for special classes of graphs such as stars, path graphs, union and join of graphs.

At this juncture, it is also relevant to compare the results proved in this paper with those proved in [23]. While we derived the implicit information inequalities by assuming certain properties for the functionals, the implicit information inequalities derived in [23] are based on certain conditions for the calculated vertex probabilities. Interestingly, note that by using Theorem (11) and Theorem (17), the range of the corresponding bounds is very small. We inferred that the difference between the upper and lower bound equals $\log_2 e \approx 1.442695$.

As noted earlier, relations between entropy-based measures for graphs have not been extensively explored so far. Apart from the results we have gained in this paper, we therefore state a few open problems as future work:

- To find relations between $I_f(G)$ and $I_f(H)$, when H is an induced subgraph of G and f is an arbitrary information functional.
- To find relations between $I_f(G)$ and $\{I_f(T_1), I_f(T_2), \ldots, I_f(T_n)\}$, where T_i, $1 \le i \le n$ are so-called generalized trees, see [34]. Note that it is always possible to decompose an arbitrary, undirected graph into a set of generalized trees [34].
- To find relations between measures based on information functionals and the other classical graph measures.
- To derive information inequalities for graph entropy measures using random graphs.
- To derive statements to judge the quality of information inequalities.

Author Contributions

Wrote the paper: MD LS. Performed the mathematical analysis: MD LS.

References

1. Basak SC (1999) Information-theoretic indices of neighborhood complexity and their applications. In: Devillers J, Balaban AT, eds. Topological Indices and Related Descriptors in QSAR and QSPAR, Gordon and Breach Science Publishers, Amsterdam, The Netherlands. pp 563–595.
2. Wang J, Provan G (2009) Characterizing the structural complexity of real-world complex networks. In: Zhou J, ed. Complex Sciences, Springer, Berlin/Heidelberg, Germany, volume 4 of *Lecture Notes of the Institute for Computer Sciences, Social Informatics and Telecommunications Engineering*. pp 1178–1189.

3. Dehmer M, Mowshowitz A (2011) A history of graph entropy measures. Information Sciences 181: 57–78.
4. Li M, Vitányi P (1997) An Introduction to Kolmogorov Complexity and Its Applications Springer.
5. Mowshowitz A (1968) Entropy and the complexity of graphs: I. an index of the relative complexity of a graph. Bulletin of Mathematical Biophysics 30: 175–204.
6. Shannon CE (1948) A mathematical theory of communication. Bell System Technical Journal 27: 379–423 and 623–656.
7. Bonchev D, Rouvray DH (2003) Complexity in chemistry: Introduction and Fundamentals. Mathematical and Computational Chemistry 7. New York: CRC Press.
8. Bonchev D (1983) Information Theoretic Indices for Characterization of Chemical Structures. Research Studies Press, Chichester.
9. Dehmer M (2008) Information processing in complex networks: graph entropy and information functionals. Appl Math Comput 201: 82–94.
10. Emmert-Streib F, Dehmer M (2007) Information theoretic measures of UHG graphs with low computational complexity. Appl Math Comput 190: 1783–1794.
11. Mehler A, Weiß P, Lücking A (2010) A network model of interpersonal alignment. Entropy 12: 1440–1483.
12. Bonchev D (2003) Complexity in Chemistry. Introduction and Fundamentals. Taylor and Francis. Boca Raton, FL, USA.
13. Anand K, Bianconi G (2009) Entropy measures for networks: Toward an information theory of complex topologies. Phys Rev E 80: 045102.
14. Costa LdF, Rodrigues FA, Travieso G, Boas PRV (2007) Characterization of complex networks: A survey of measurements. Advances in Physics 56: 167–242.
15. Kim J, Wilhelm T (2008) What is a complex graph? Physica A: Statistical Mechanics and its Applications 387: 2637–2652.
16. Balaban AT, Balaban TS (1991) New vertex invariants and topological indices of chemical graphs based on information on distances. Journal of Mathematical Chemistry 8: 383–397.
17. Bertz SH (1983) A mathematical model of complexity. In: King R, ed. Chemical applications of topology and graph theory, Elsevier, Amsterdam. pp 206–221.
18. Basak SC, Magnuson VR, Niemi GJ, Regal RR (1988) Determining structural similarity of chemicals using graph-theoretic indices. Discrete Applied Mathematics 19: 17–44.
19. Bonchev D, Rouvray DH (2005) Complexity in chemistry, biology, and ecology. Mathematical and Computational Chemistry. New York: Springer. pp xx+344. doi:10.1007/b136300. URL http://dx.doi.org/10.1007/b136300.
20. Claussen JC (2007) Offdiagonal complexity: A computationally quick complexity measure for graphs and networks. Physica A: Statistical Mechanics and its Applications 375: 365–373.
21. Körner J (1973) Coding of an information source having ambiguous alphabet and the entropy of graphs. Trans 6th Prague Conference on Information Theory. pp 411–425.
22. Butts C (2001) The complexity of social networks: Theoretical and empirical findings. Social Networks 23: 31–71.
23. Dehmer M, Mowshowitz A (2010) Inequalities for entropy-based measures of network information content. Applied Mathematics and Computation 215: 4263–4271.
24. Dehmer M, Mowshowitz A, Emmert-Streib F (2011) Connections between classical and parametric network entropies. PLoS ONE 6: e15733.
25. Bonchev D, Trinajstic N (1977) Information theory, distance matrix, and molecular branching. The Journal of Chemical Physics 67: 4517–4533.
26. Dehmer M, Borgert S, Emmert-Streib F (2008) Entropy bounds for hierarchical molecular networks. PLoS ONE 3: e3079.
27. Skorobogatov VA, Dobrynin AA (1988) Metrical analysis of graphs. MATCH Commun Math Comp Chem 23: 105–155.
28. Shannon C, Weaver W (1997) The Mathematical Theory of Communication. University of Illinois Press, Urbana, IL, USA.
29. Freeman LC (1977) A set of measures of centrality based on betweenness. Sociometry 40: 35–41.
30. Freeman LC (1978) Centrality in social networks conceptual clarification. Social Networks 1: 215–239.
31. Sabidussi G (1966) The centrality index of a graph. Psychometrika 31: 581–603.
32. Emmert-Streib F, Dehmer M (2011) Networks for systems biology: Conceptual connection of data and function. IET Systems Biology 5: 185–207.
33. Simonyi G (1995) Graph entropy: A survey. In: Cook W, Lovász L, Seymour P, eds. Combinatorial Optimization, DIMACS Series in Discrete Mathematics and Theoretical Computer Science, volume 20. pp 399–441.
34. Emmert-Streib F, Dehmer M, Kilian J (2006) Classification of large graphs by a local tree decomposition. In:, , et al HRA, editor (2006) Proceedings of DMIN'05, International Conference on Data Mining, Las Vegas, USA. pp 477–482.