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INFORMATION INEQUALITIES FOR GRAPHS

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Abstract: *In this paper, we state information inequalities for nanostructures representing graphs by using some novel information functionals. We use a recently proposed approach to determine the structural information content of arbitrary undirected and connected graphs. In contrast to the information indices often used in chemical information theory, the entropy measure does not depend on the problem to determine vertex partitions of a graph under consideration. Finally, to define the entropy of a graph, we use certain information functionals. As the main result, we derive so - called implicit and explicit information inequalities for arbitrary undirected and connected graphs.*

Keywords: Undirected Graphs; Nanostructures; Chemical Graphs; Symmetry; Structural Information Content; Graph Entropy; Information Theory.

1. INTRODUCTION

So far, several classes of nanostructures representing (chemical) graphs by using graph - theoretical indices which characterize structural features of the underlying graphs have been frequently investigated, e.g., see (Ashrafi, Ghorbani and Jalali, 2008; Diudea, Stefu, Parv and John, 2004; Diudea and Nagy, 2007; Yousefi - Azari, Ashrafi and Khalifeh, 2008). Generally, to characterize chemical graphs topologically, various topological indices have been used (Devillers and Balaban, 1999). An interesting class of such indices for characterizing networks are information measures (Bonchev, 1983; Bonchev, 1979; Emmert - Streib and Dehmer, 2007) which are usually based on the well known SHANNON - entropy (Shannon and Weaver, 1997). Mathematical properties of such information measures for graphs have been intensely investigated in (Bonchev, 1983; Bonchev, 1979; Devillers and Balaban, 1999; Solé and Valverde, 2004).

In this paper, we discuss the problem of deriving information inequalities for arbitrary undirected and connected networks. In information theory, the problem of investigating information inequalities has been addressed by (Zhang and Yeung, 1997; Zhang and Yeung, 1998). In contrast, we express some implicit and explicit information inequalities for graphs. The problem of finding implicit information inequalities has been already similarly addressed in (Dehmer, 2008; Dehmer, Borgert and Emmert - Streib, 2008). To derive the corresponding graph entropy measures by using some novel information functionals, we use an approach that has been recently discussed in (Dehmer, 2008). As the main contribution of this paper, we obtain some implicit and explicit information inequalities for graphs based on the defined information functionals.

It is important to mention that in this paper, we will not interpret the derived entropy measures explicitly based on sets of chemical graphs. We already investigated the meaning of some these graph entropy measures (based on the information functional $f^S(v_i)$ and similar ones) in (Dehmer and Emmert - Streib, 2008; Dehmer, Varmuza, Borgert and Emmert - Streib, 2009). Especially by using the information functional $f^S(v_i)$, we found that a similarly defined graph entropy measure (see (Dehmer, Varmuza, Borgert and Emmert - Streib, 2009)) characterizes the diversity of the atoms in terms of neighborhoods, and thereby captures a special type of structural complexity and inner symmetry (Dehmer, Varmuza, Borgert and Emmert - Streib, 2009). Of course, such insights could be obtained by considering the information functionals we will define in the present paper. However, this will not be the point of this paper. As mentioned above, we focus on deriving information inequalities based on the novel information functionals we will introduce.

2. INFORMATION MEASURES IN CHEMICAL INFORMATION THEORY

In the following, we give a short review of such information measures for graphs which have been intensely used in chemical information theory. The rich variety of molecular structures contributed to the considerable efforts to introduce information measures of graphs (Bonchev, 1983; Bonchev, Mekenyan and Trinajstić, 1981; Bonchev and Trinajstić, 1982; Bonchev, 1995; Bonchev, 2003; Bonchev and Buck, 2005). The Shannon equations can be more generally treated for characterizing the distribution of any graph invariant X according to a certain equivalency criterion α:

$$I(G,\alpha) = |X|\log(|X|) - \sum_{i=1}^{k} |X_i|\log(|X_i|), \qquad (1)$$

$$\bar{I}(G,\alpha) = -\sum_{i=1}^{k} P_i \log(P_i) = -\sum_{i=1}^{k} \frac{|X_i|}{|X|}\log\left(\frac{|X_i|}{|X|}\right). \qquad (2)$$

The first invariant studied was the number of graph vertices, while the equivalence criterion α, which produces the vertex set partitioning into k subsets of cardinality $|V_i|$, included vertex coloring (elemental composition of molecule), vertex degree denoted by $\delta(v_i)$ (Harary, 1969), extended (second, third, etc.) vertex degree (Basak, 1987) and its combining with the elementary composition (the RASHESVSKY approach (Rashevsky, 1955)), orbits of the vertex automorphisms group of the graph (Trucco, 1956), vertex total distance (Bonchev and Trinajstić, 1977), and vertex ordering with respect to the graph center (Bonchev, Balaban and Mekenyan, 1980). Later, RASHESVSKY's approach has been more rigorously treated as an extension of the finite probability scheme by MOWSHOWITZ (Mowshowitz, 1968), and applied to other important graph invariant decompositions.

One of the latest graph complexity measures is based on the distribution of the vertex degree to distance ratios, $b_i = \frac{\delta(v_i)}{d_i}$ (Bonchev and Buck, 2005), an information functional, which integrates two of the criteria for a complex graph – high connectivity and small radius. The possibility for using the number of graph edges $|E|$ as a basis for additional information functionals has been first mentioned by TRUCCO (Trucco, 1956), who proposed to use the graph edges partitioning into the orbits of the edge automorphisms group of the graph.

A more sophisticated information measure has been developed recently within the framework of the overall topological indices concept (Bonchev, 2005). It calculates the overall value OX of a certain graph invariant X by summing up its values in all subgraphs, and partitioning them into terms of increasing orders. Many concrete measures can be found in (Bonchev, 2005). The properties of most of the here mentioned information functionals are not studied in detail, and will be a subject of our future research.

3. INFORMATION FUNCTIONALS

In this section, we define some novel information functionals for graphs. Starting from these functionals, we obtain families of entropic measures. In this paper, we restrict our analysis to undirected and connected graphs without loops and multiple edges. Before starting with the definitions, we first express the required graph - theoretical preliminaries (Harary, 1969; Skorobogatov and Dobrynin, 1988). Let $\mathcal{G}_{UC}$ be the set of finite, undirected and connected graphs $G = (V, E)$. $K_{|V|}$ denotes the complete graph with $|V|$ vertices. The degree of a vertex $v \in V$ is denoted by $\delta(v)$ and equals the number of edges $e \in E$ which are incident with v. The quantity $\sigma(v) = \max_{u \in V} d(u, v)$ is called the eccentricity of $v \in V$. $d(u, v)$ denotes the shortest distance between u and v. $\rho(G) = \max_{v \in V} \sigma(v)$ and $r(G) = \min_{v \in V} \sigma(v)$ is called the diameter and the radius of G, respectively. Further, we define

$$S_j(v_i) := \{v \in V \,|\, d(v_i, v) = j,\ j \geq 1\}. \qquad (3)$$

$S_j(v_i)$ is called j - sphere of v_i regarding G. In the following, we use the definition of the so - called local information graph $L(v_i, j)$ of $G \in \mathcal{G}_{UC}$ that has been originally defined in (Dehmer, 2008). This definition is used to define information functionals we want to use in this paper. For a vertex $v_i \in V$, we set $S_j(v_i) = \{v_{u_j}, v_{w_j}, \ldots, v_{x_j}\}$ and determine the induced shortest paths:

$$\begin{aligned} P_1^j(v_i) &= (v_i, v_{u_1}, v_{u_2}, \ldots, v_{u_i}), && (4)\\ P_2^j(v_i) &= (v_i, v_{w_1}, v_{w_2}, \ldots, v_{w_j}), && (5)\\ &\vdots \\ P_{k_j}^j(v_i) &= (v_i, v_{x_1}, v_{x_2}, \ldots, v_{x_j}). && (6) \end{aligned}$$

The corresponding edge sets are defined by

$$E_1^j = \{\{v_i, v_{u_1}\}, \{v_{u_1}, v_{u_2}\}, \{v_{u_2}, v_{u_3}\}, \ldots, \{v_{u_{j-1}}, v_{u_j}\}\}, \qquad (7)$$

$$E_2^j = \{\{v_i, v_{w_1}\}, \{v_{w_1}, v_{w_2}\}, \{v_{w_2}, v_{w_3}\}, \dots, \{v_{w_{j-1}}, v_{w_j}\}\}, \quad (8)$$

$$\vdots \qquad \vdots$$

$$E_{k_j}^j = \{\{v_i, v_{x_1}\}, \{v_{x_1}, v_{x_2}\}, \{v_{x_2}, v_{x_3}\}, \dots, \{v_{x_{j-1}}, v_{x_j}\}\}. \quad (9)$$

If we now set
$V_L^j := \{v_i, v_{u_1}, v_{u_2}, \dots, v_{u_j}\} \cup \{v_i, v_{w_1}, v_{w_2}, \dots, v_{w_j}\} \cup \dots \cup \{v_i, v_{x_1}, v_{x_2}, \dots, v_{x_j}\}$,

and $E_L^j := E_1^j \cup E_2^j \cup \dots \cup E_{k_j}^j$, we define the local information graph $L(v_i, j)$ of G regarding v_i by

$$L(v_i, j) = (V_L^j, E_L^j). \quad (10)$$

We remark that the local information graph regarding $v_i \in V$ can not always be uniquely defined because there often exists more than one path from v_i to a certain vertex in the corresponding j - sphere (Dehmer, 2008).

Definition 3.1 Let $G = (V, E) \in \mathcal{G}_{UC}$. *We define the information functional* $f^S(v_i)$ *by*

$$f^S(v_i) := c_1|S_1(v_i)| + c_2|S_2(v_i)| + \dots + c_{\rho(G)}|S_{\rho(G)}(v_i)|, \quad (11)$$

where the $c_k,\ 1 \le k \le \rho(G)$ are real positive coefficients.

Definition 3.2 Let $G = (V, E) \in \mathcal{G}_{UC}$. *We define the information functional* $f^d(v_i)$ *by*

$$f^d(v_i) := d(v_i, v_1) + d(v_i, v_2) + \dots + d(v_i, v_{|V|}). \quad (12)$$

Definition 3.3 Let $G = (V, E) \in \mathcal{G}_{UC}$. *We define the information functional* $f^E(v_i)$ *by*

$$f^E(v_i) := b_1|E(L(v_i, 1))| + b_2|E(L(v_i, 2))| + \dots + b_{\rho(G)}|E(L(v_i, \rho(G)))|, \quad (13)$$

where the $b_k,\ 1 \le k \le \rho(G)$ *are real positive coefficients.* $|E(L(v_i, j))|$ *denotes the number of edges of* $L(v_i, j)$.

Definition 3.4 *Let* $G = (V, E) \in \mathcal{G}_{UC}$. *For each vertex* $v_i \in V$, *we define the vertex probabilities as follows*

$$p^{f^S}(v_i) := \frac{f^S(v_i)}{\sum_{j=1}^{|V|} f^S(v_j)}, \qquad (14)$$

$$p^{f^d}(v_i) := \frac{f^d(v_i)}{\sum_{j=1}^{|V|} f^d(v_j)}, \qquad (15)$$

and

$$p^{f^E}(v_i) := \frac{f^E(v_i)}{\sum_{j=1}^{|V|} f^E(v_j)}. \qquad (16)$$

Definition 3.5 *We finally define the corresponding entropic measures by*

$$I^{f^S}(G) := -\sum_{i=1}^{|V|} \frac{f^S(v_i)}{\sum_{j=1}^{|V|} f^S(v_j)} \log\left(\frac{f^S(v_i)}{\sum_{j=1}^{|V|} f^S(v_j)}\right), \qquad (17)$$

$$I^{f^d}(G) := -\sum_{i=1}^{|V|} \frac{f^d(v_i)}{\sum_{j=1}^{|V|} f^d(v_j)} \log\left(\frac{f^d(v_i)}{\sum_{j=1}^{|V|} f^d(v_j)}\right), (18)$$

and

$$I^{f^E}(G) := -\sum_{i=1}^{|V|} \frac{f^E(v_i)}{\sum_{j=1}^{|V|} f^E(v_j)} \log\left(\frac{f^E(v_i)}{\sum_{j=1}^{|V|} f^E(v_j)}\right). \qquad (19)$$

A simple observation for finding graphs which maximize these entropic measures represents the following statement.

Theorem 3.1 *The complete graph $K_{|V|}$ maximizes $I^f(G)$ by using the information functionals $f^S(v_i), f^d(v_i)$, and $f^E(v_i)$.*

Proof: We start the information functional $I^{f^E}(G)$. For each vertex v_i of $K_{|V|}$, it holds $|E(L(v_i,1))| = |V| - 1$ and $|E(L(v_i,j))| = 0,\ 2 \leq j \leq \rho(G)$. Hence, we yield

$$p^{f^E}(v_i) := \frac{b_1(|V|-1)}{|V|(|V|-1)b_1} = \frac{1}{|V|}. \qquad (20)$$

Therefore, $I^{f^E}(K_{|V|})$ attains maximum entropy. For $f^S(v_i)$ and $f^d(v_i)$, the proof can be done analogously.

4. INFORMATION INEQUALITIES

In this section, we prove some information inequalities for graphs. In this paper, we divide the obtained information inequalities into the following two categories:

1. Implicit information inequalities: The entropy of a graph G is characterized by another graph entropy expression based on an inequality
(Example: $I^f(G) \underset{(>)}{<} \alpha I^{f^\star}(G)$).
2. Explicit information inequalities: The entropy of a graph G will be estimated by a constant expression (Example: $I^f(G) \underset{(>)}{<} \beta$.)

4.1. IMPLICIT INFORMATION INEQUALITIES

We start this section with expressing an assertion to obtain certain information inequalities for graphs. This assertion has been already expressed in (Dehmer, 2008) for deriving relationships between the resulting graph entropies by using different parameterized information functionals (Dehmer, 2008).

Lemma 4.1 *Let $G \in \mathcal{G}_{UC}$. Further, let f and $f^\star$ be two arbitrary information functionals. If the relation*

$$p^f(v_i) \underset{(>)}{<} \alpha p^{f^\star}(v_i), \qquad (21)$$

holds, then we obtain

$$I^f(G) \underset{(<)}{>} \alpha I^{f^\star}(G) - \alpha \log(\alpha). \qquad (22)$$

Either, α depends from the information functionals or is a constant expression.

By using this lemma, we are now able to state implicit information inequalities according to the defined information functionals.

Theorem 4.1 *Let $G \in \mathcal{G}_{UC}$. Let f^S and f^d be the information functionals expressed by Definition (3.1) and Definition (3.2), respectively. First, the inequality*

$$p^{f^S}(v_i) < p^{f^d}(v_i)\varphi^c\rho(G)\frac{\sum_{j=1}^{|V|} f^d(v_j)}{\sum_{j=1}^{|V|} f^S(v_j)}, \qquad (23)$$

is valid, where $\varphi^c := \max_{1\leq j\leq \rho} c_j$. Second, it holds

$$I^{f^S}(G) > \varphi^c\rho(G)\frac{\sum_{j=1}^{|V|} f^d(v_j)}{\sum_{j=1}^{|V|} f^S(v_j)} I^{f^d}(G) - \varphi^c\rho(G)\frac{\sum_{j=1}^{|V|} f^d(v_j)}{\sum_{j=1}^{|V|} f^S(v_j)} \log\left(\varphi^c\rho(G)\frac{\sum_{j=1}^{|V|} f^d(v_j)}{\sum_{j=1}^{|V|} f^S(v_j)}\right). \qquad (24)$$

Proof: For deriving a relation between $f^S(v_i)$ and $f^d(v_i)$, we first observe that

$$|S_j(v_i)| \leq d(v_i, v_1) + d(v_i, v_2) + \cdots + d(v_i, v_{|V|}) = f^d(v_i), \qquad (25)$$

holds. To see this inequality, we always find

$$\begin{aligned} \gamma = |S_j(v_i)| &\leq \gamma \cdot j + \sum_{v \notin S_j(v_i)} d(v_i, v), \\ &= \sum_{v \in S_j(v_i)} d(v_i, v) + \sum_{v \notin S_j(v_i)} d(v_i, v), \\ &= d(v_i, v_1) + d(v_i, v_2) + \cdots + d(v_i, v_{|V|}), \quad \gamma, j \geq 1. \qquad (26) \end{aligned}$$

Hence, Inequality (25) holds. If we now assume that at least two consecutive coefficients are not equal, we further obtain

$$\begin{aligned} f^S(v_i) &:= c_1|S_1(v_i)| + c_2|S_2(v_i)| + \cdots + c_{\rho(G)}|S_{\rho(G)}(v_i)| \\ &< \varphi^c\left(|S_1(v_i)| + |S_2(v_i)| + \cdots + |S_{\rho(G)}(v_i)|\right) \\ &\leq \varphi^c\rho(G)f^d(v_i). \qquad (27) \end{aligned}$$

From this, we yield

$$\begin{aligned} p^{f^S}(v_i) = \frac{f^S(v_i)}{\sum_{j=1}^{|V|} f^S(v_j)} &< \varphi^c\rho(G)\frac{f^d(v_i)}{\sum_{j=1}^{|V|} f^S(v_j)}, \\ &= p^{f^d}(v_i)\varphi^c\rho(G)\frac{\sum_{j=1}^{|V|} f^d(v_j)}{\sum_{j=1}^{|V|} f^S(v_j)}. \qquad (28) \end{aligned}$$

By setting $\alpha := \varphi^c \rho(G) \frac{\sum_{j=1}^{|V|} f^d(v_j)}{\sum_{j=1}^{|V|} f^S(v_j)}$ and applying Lemma (4.1), we now infer Inequality (24). Hence, the theorem is proven.

Theorem 4.2 *Let $G \in \mathcal{G}_{UC}$. It holds*

$$I^{f^S}(G) > \varphi^c \frac{\varphi^c}{\phi^c} |V| \rho(G) I^{f^d}(G) - \frac{\varphi^c}{\phi^c} |V| \rho(G) \log\left(\frac{\varphi^c}{\phi^c} |V| \rho(G)\right), \tag{29}$$

where $\phi^c := \min_{1 \le j \le \rho} c_j$.

Proof: We start with Inequality (23). By estimating the fraction of this inequality, we yield

$$\begin{aligned} p^{f^S}(v_i) < p^{f^d}(v_i) \varphi^c \rho(G) \frac{\sum_{j=1}^{|V|} f^d(v_j)}{\sum_{j=1}^{|V|} f^S(v_j)} &< p^{f^d}(v_i) \varphi^c \rho(G) \frac{|V|^2 \rho(G)}{|V| \phi^c \rho(G)}, \\ &= p^{f^d}(v_i) \frac{\varphi^c}{\phi^c} |V| \rho(G), \end{aligned} \tag{30}$$

because it holds

$$\begin{aligned} \sum_{j=1}^{|V|} f^d(v_j) &= \sum_{j=1}^{|V|} \left(d(v_j, v_1) + d(v_j, v_2) + \cdots + d(v_j, v_{|V|})\right) \\ &< \sum_{j=1}^{|V|} |V| \rho(G) = |V|^2 \rho(G), \end{aligned} \tag{31}$$

and

$$\begin{aligned} \sum_{j=1}^{|V|} f^S(v_j) &= \sum_{j=1}^{|V|} \left(c_1 |S_1(v_i)| + c_2 |S_2(v_i)| + \cdots + c_{\rho(G)} |S_{\rho(G)}(v_i)|\right) \\ &> \sum_{j=1}^{|V|} \phi^c \rho(G) = |V| \phi^c \rho(G). \end{aligned} \tag{32}$$

Now, by applying Lemma (4.1), we infer Inequality (29).

Theorem 4.3 *Let $G \in \mathcal{G}_{UC}$. Further, we define*

$$\varphi^c := \max_{1\le j\le\rho} c_j \quad \text{and} \quad \omega(v_i) := \max_{1\le j\le\rho} |S_j(v_i)|.$$

First, the inequality

$$p^{f^S}(v_i) < p^a(v_i)\frac{\sum_{j=1}^{|V|} a(v_j)}{\sum_{j=1}^{|V|} f^S(v_j)}, \qquad (33)$$

is valid, where $p^a(v_i) := \frac{a(v_i)}{\sum_{j=1}^{|V|} a(v_j)}$ *and* $a(v_i) := \varphi^c \cdot \rho(G) \cdot \omega(v_i)$*. Second, it holds*

$$I^{f^S}(G) > \frac{\sum_{j=1}^{|V|} a(v_j)}{\sum_{j=1}^{|V|} f^S(v_j)} I^a(G) - \frac{\sum_{j=1}^{|V|} a(v_j)}{\sum_{j=1}^{|V|} f^S(v_j)} \log\left(\frac{\sum_{j=1}^{|V|} a(v_j)}{\sum_{j=1}^{|V|} f^S(v_j)}\right). \quad (34)$$

Proof: Starting from the definition of the information functional f^S, we get the estimation

$$\begin{aligned} f^S(v_i) &:= c_1|S_1(v_i)| + c_2|S_2(v_i)| + \cdots + c_{\rho(G)}|S_{\rho(G)}(v_i)| \\ &< \varphi^c \cdot \rho(G) \cdot \omega(v_i) =: a(v_i). \end{aligned} \qquad (35)$$

From this, we yield

$$p^{f^S}(v_i) = \frac{f^S(v_i)}{\sum_{j=1}^{|V|} f^S(v_j)} < \frac{a(v_i)}{\sum_{j=1}^{|V|} a(v_j)} \cdot \frac{\sum_{j=1}^{|V|} a(v_j)}{\sum_{j=1}^{|V|} f^S(v_j)} = p^a(v_i) \cdot \frac{\sum_{j=1}^{|V|} a(v_j)}{\sum_{j=1}^{|V|} f^S(v_j)}. \quad (36)$$

Once again, by now applying Lemma (4.1), one finalizes the proof of Theorem (4.3).

Theorem 4.4 *Let* $G \in \mathcal{G}_{UC}$*. It holds*

$$I^{f^S}(G) > \frac{\varphi^c}{\phi^c}\omega I^a(G) - \frac{\varphi^c}{\phi^c}\omega \log\left(\frac{\varphi^c}{\phi^c}\omega\right), \qquad (37)$$

where $\omega := \max_{1\le i\le|V|} \omega(v_i)$*.*

Proof: We see that

$$p^{f^S}(v_i) < p^a(v_i) \cdot \frac{\sum_{j=1}^{|V|} a(v_j)}{\sum_{j=1}^{|V|} f^S(v_j)} < p^a(v_i) \cdot \frac{\varphi^c}{\phi^c}\omega \qquad (38)$$

holds, because we obtain

$$\sum_{j=1}^{|V|} a(v_j) < |V| \cdot \varphi^c \cdot \rho(G) \cdot \omega, \qquad (39)$$

and

$$\sum_{j=1}^{|V|} f^S(v_j) > |V| \cdot \phi^c \cdot \rho(G). \quad (40)$$

Now, the application of Lemma (4.1) to Inequality (38) completes the proof.

To finalize this section, we also want to express an implicit information inequality by incorporating $f^E(v_i)$ and $f^S(v_i)$.

Theorem 4.5 *Let $G \in \mathcal{G}_{UC}$. If it holds $c_i \leq b_i$, then we yield*

$$I^{f^S}(G) > \frac{\sum_{j=1}^{|V|} f^E(v_j)}{\sum_{j=1}^{|V|} f^S(v_j)} I^{f^E}(G) - \frac{\sum_{j=1}^{|V|} f^E(v_j)}{\sum_{j=1}^{|V|} f^S(v_j)} \log\left(\frac{\sum_{j=1}^{|V|} f^E(v_j)}{\sum_{j=1}^{|V|} f^S(v_j)}\right). \quad (41)$$

Proof: We do give a sketch of this proof only. The main step is to find a relation between $f^E(v_i)$ and $f^S(v_i)$. Now, we infer that it generally holds

$$\begin{aligned} |S_j(v_i)| \leq j + |S_j(v_i)| - 1 &\leq j + |S_j(v_i)| - 1 + x, \quad j \geq 1,\ x \geq 0 \\ &= |E(L(v_i, j))|. \end{aligned} \qquad (42)$$

Starting from Inequality (42) and taking $c_i \leq b_i$ into account, we further get

$$p^{f^S}(v_i) < \frac{\sum_{j=1}^{|V|} f^E(v_j)}{\sum_{j=1}^{|V|} f^S(v_j)} p^{f^E}(v_i). \qquad (43)$$

By now applying Lemma (4.1) to Inequality (43), the proof can be completed.

Remark 4.1 *We want to remark that many other implicit information inequalities can be proven. In summary, the shown method mainly depends on (i) finding certain relationships between the information functionals which capture structural information* *of a graph (e.g., see Theorem (4.1)) or (ii) finding estimations for the used information functionals (e.g., see Theorem (4.3)).*

4.2. EXPLICIT INFORMATION INEQUALITIES

As a first attempt, we state some explicit information inequalities based on the information functionals we have expressed in Section(3).

Theorem 4.6 *Let $G \in \mathcal{G}_{UC}$. We define*

$$\varphi_i^b := \max_{\substack{1\leq j\leq \rho \\ j\neq i}} b_j,\ \phi_i^b := \min_{\substack{1\leq j\leq \rho \\ j\neq i}} b_j,\ \varphi_i^c := \max_{\substack{1\leq j\leq \rho \\ j\neq i}} c_j,\ \phi_i^c := \min_{\substack{1\leq j\leq \rho \\ j\neq i}} c_j, \quad (44)$$

$$\omega_i := \max_{\substack{1\leq j\leq |V| \\ j\neq i}} \omega(v_j). \quad (45)$$

Then, the following inequalities are valid:

$$I^{f^S}(G) > \left|p^{f^S}(v_i)\log\left(p^{f^S}(v_i)\right)\right| - \left(|V|-1\right)\left|\frac{\varphi_i^c\cdot\omega}{\phi_i^c\cdot|V|}\log\left(\frac{\phi_i^c}{\varphi_i^c\cdot|V|\cdot\omega}\right)\right|, \quad (46)$$

$$I^{f^d}(G) > \left|p^{f^d}(v_i)\log\left(p^{f^d}(v_i)\right)\right| - \left(|V|-1\right)\left|\frac{\rho(G)}{|V|}\log\left(\frac{1}{|V|\rho(G)}\right)\right|, \quad (47)$$

and

$$I^{f^E}(G) > \left|p^{f^E}(v_i)\log\left(p^{f^E}(v_i)\right)\right| - \left(|V|-1\right)\left|\frac{\varphi_i^b\cdot|E|}{\phi_i^b\cdot|V|}\log\left(\frac{\phi_i^b}{\varphi_i^b\cdot|V|\cdot|E|}\right)\right|. \quad (48)$$

Proof: To prove Inequality (46), we find

$$\begin{aligned}
I^{f^S}(G) &:= -\sum_{i=1}^{|V|}\frac{f^S(v_i)}{\sum_{j=1}^{|V|}f^S(v_j)}\log\left(\frac{f^S(v_i)}{\sum_{j=1}^{|V|}f^S(v_j)}\right),\\
&= \sum_{i=1}^{|V|}\left|\frac{f^S(v_i)}{\sum_{j=1}^{|V|}f^S(v_j)}\log\left(\frac{f^S(v_i)}{\sum_{j=1}^{|V|}f^S(v_j)}\right)\right|,\\
&> \left|p^{f^S}(v_i)\log\left(p^{f^S}(v_i)\right)\right| - \sum_{\substack{j=1\\ j\neq i}}^{|V|}\left|\frac{f^S(v_i)}{\sum_{j=1}^{|V|}f^S(v_j)}\log\left(\frac{f^S(v_i)}{\sum_{j=1}^{|V|}f^S(v_j)}\right)\right|. \quad (49)
\end{aligned}$$

Further, we yield

$$\frac{f^S(v_i)}{\sum_{j=1}^{|V|} f^S(v_j)} > \frac{\phi_i^c}{\varphi_i^c \cdot \sum_{j=1}^{|V|} \omega(v_j)} > \frac{\phi_i^c}{\varphi_i^c \cdot |V| \cdot \omega}, \quad (50)$$

and

$$\frac{f^S(v_i)}{\sum_{j=1}^{|V|} f^S(v_j)} < \frac{\varphi_i^c \cdot \omega}{\phi_i^c \cdot |V|}. \quad (51)$$

Now, we finally infer

$$I^{f^S}(G) > \left|p^{f^S}(v_i) \log\left(p^{f^S}(v_i)\right)\right| - \left(|V|-1\right)\left|\frac{\varphi_i^c \cdot \omega}{\phi_i^c \cdot |V|} \log\left(\frac{\phi_i^c}{\varphi_i^c \cdot |V| \cdot \omega}\right)\right|. \quad (52)$$

But this inequality equals Inequality (46). Inequality (47) and Inequality (48) can be proven analogously.

The following theorem can be similarly proven than Theorem (4.6).

Theorem 4.7 *Let* $G \in \mathcal{G}_{UC}$*. We define* $\varphi^b := \max_{1 \le j \le \rho} b_j$ *and* $\phi^b := \min_{1 \le j \le \rho} b_j$*. Then, the following inequalities are valid:*

$$I^{f^S}(G) < |V| \left|\frac{\varphi^c \cdot \omega}{\phi^c \cdot |V|} \log\left(\frac{\phi^c}{\varphi^c \cdot |V| \cdot \omega}\right)\right|, \quad (53)$$

$$I^{f^d}(G) < |V| \left|\frac{\varphi^c \cdot \omega}{\phi^c \cdot |V|} \log\left(\frac{\phi^c}{\varphi^c \cdot |V| \cdot \omega}\right)\right|, \quad (54)$$

and

$$I^{f^E}(G) < |V| \left|\frac{\varphi^b \cdot |E|}{\phi^b \cdot |V|} \log\left(\frac{\phi^b}{\varphi^b \cdot |V| \cdot |E|}\right)\right|. \quad (55)$$

5. SUMMARY AND CONCLUSION

In this paper, we investigated the problem of deriving information inequalities for graphs. For doing so, we used the construction of the graph entropy measure which has been published in (Dehmer, 2008). Here, we distinguished so called implicit and explicit information inequalities (see Section 4). For example, the proven inequalities may serve for characterizing graphs, e.g., see (Dehmer, Borgert and Emmert - Streib, 2008). For deriving implicit inequalities, either one has to infer a relation between the used information functionals under consideration or one must find an estimation for an information functional that quantifies structural information of a graph. In contrast, explicit information inequalities represent estimates for the entropies of graphs (e.g., representing lower or upper bounds).

As future work, we want to define further information functionals to characterize certain graph classes by using entropy measures. In particular, we would like to infer information inequalities for classical entropy measures used in chemical graph theory by investigating the corresponding information functional in depth. Such relations are almost unexplored so far. Further, we want to work towards the challenging problem of interpreting the derived information inequalities for given sets of anostructures representing chemical graphs. Another point of interest is to interpret the introduced information measures (based on the defined information functionals) with respect to given sets of nanostructures.

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