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Information processing in complex networks: Graph entropy and information functionals

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Abstract

This paper introduces a general framework for defining the entropy of a graph. Our definition is based on a local information graph and on information functionals derived from the topological structure of a given graph. More precisely, an information functional quantifies structural information of a graph based on a derived probability distribution. Such a probability distribution leads directly to an entropy of a graph. Then, the structural information content of a graph will be is interpreted and defined as the derived graph entropy. Another major contribution of this paper is the investigation of relationships between graph entropies. In addition to this, we provide numerical results demonstrating not only the feasibility of our method, which has polynomial time complexity, but also its usefulness with regard to practical applications aiming to an understanding of information processing in complex networks.

Keywords: Graphs; Structural information content; Graph entropy; Information theory; Applied graph theory

1. Introduction

Entropy-based methods are powerful tools to investigate various problems in, e.g., mathematical chemistry, cybernetics, computational physics and pattern recognition [3,18,16,23,28,35]. Particularly, the application of information-theoretical methods to analyze graph-based systems is currently of considerable interest [6,7,9,14,22]. For example, in chemical graph theory [12,32] there are many approaches to characterize molecular structures based on so called information indices [3]. The determination of the structural information content [3,24–27,29,33] of a graph is also a classical problem in the areas mentioned above. Thereby, classical methods to compute the structural information content of a graph are mostly based on finding a certain partitioning of the vertex set to obtain a probability distribution [24–27,29,33]. Based on such a probability distribution derived from a vertex partitioning, the entropy of a graph can be defined. In this context, the structural information content is defined as the entropy of the underlying graph topology. Another classical

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definition of graph entropy that is rooted in information theory was orginally introduced in [21]. In contrast to these classical approaches, in this paper we first generalize the approach of [9] to define an entropy of a network by using the novel concept of the local information graph. The main idea of this graph entropy approach recently presented in [9] was to avoid the problem of determining certain vertex partitions for defining the entropy of a graph. Then, in order to define the probability value for each vertex and, hence, the entropy of a graph, local vertex functionals have been used [9]. In this paper, we will generalize this concept by introducing some novel definitions to use general structural properties or graph measures for defining information functionals for networks. Generally, information functionals for graphs can be used to quantify structural information based on a given probability distribution. However, starting from different information functionals, the investigation of relationships between the associated graph entropies is important. As one main result, we state inequalities which express relationships between the vertex probability values and the resulting graph entropies. We want to emphasize that such results are very useful to compare the entropies of certain graph classes numerically. Moreover, this paper wants to contribute to the problem of analyzing and understanding information processing in complex networks [13,15], e.g., signaling, metabolic or protein networks, by using information-theoretical methods. Another main contribution of this paper are numerical results. First, we visualize all key steps of our procedure by appropriate numerical examples and, second, we demonstrate the feasibility and usefulness of the introduced method with regard to some given graphs. It is important to note, that only methods that are computationally efficient do have the potential for practical applications. This was a major problem of some classical approaches [26,27,29,33]. However, as we demonstrate in Section 2.3, our approach has polynomial time complexity.

This paper is organized as follows: in Section 2, we introduce important definitions to generalize the graph entropy concept of [9]. Further, we define novel information functionals and briefly analyze the computational complexity to compute the resulting graph entropies. In Section 3, we state assertions for deriving relationships between the resulting graph entropies. In Section 4, we present numerical results to study the influence of different information functionals on the resulting entropies. The paper finishes in Section 5 with a summary and conclusion.

2. Quantifying structural information in networks

The goal of this section is to generalize the graph entropy method recently presented in [9] by defining the concept of the local information graph of a certain vertex $v_i \in V$. Then, by using this definition, several structural properties or graph measures can be used to define the entropy of a graph via an information functional. The steps to generalize the method of [9] can be expressed as follows:

- Definition of certain local subgraphs based on determining vertex spheres. The vertex spheres are sets of vertices whose elements have a certain shortest distance to a chosen vertex in a given graph.
- Definition of a local information radius by using a general information functional f. Then, this definition is based on the obtained local subgraphs. f quantifies structural information of the underlying graph regarding a vertex v_i.

To introduce the novel definitions, we first repeat some basic graph-theoretical preliminaries [5,17,20,31]. We remark that in this paper we throughout deal with undirected and connected graphs without loops and multiple edges.

Definition 2.1. $G = (V, E),\ |V| < \infty$ denotes a finite undirected graph, where $E \subseteq \binom{V}{2}$. G is called connected if for arbitrary vertices v_i and v_j there exists an undirected path from v_i to v_j. $\mathcal{G}_{UC}$ denotes the set of finite, undirected and connected graphs.

Definition 2.2. Let $G = (V, E) \in \mathcal{G}_{UC}$. $d(u, v)$ denotes the shortest distance between $u \in V$ and $v \in V$ where d is a metric. The quantity $\sigma(v) = \max_{u \in V} d(u, v)$ is called eccentricity of 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.

The following definitions form the key concept for using arbitrary information functionals to measure the entropy of graphs. By applying these definitions, we will see that this concept can be understood as a first attempt to investigate the local information spread [10] in complex networks.

Definition 2.3. Let $G = (V, E) \in \mathscr{G}_{UC}$. The set

$$S_j(v_i, G) := \{v \in V | d(v_i, v) = j,\ j \geqslant 1\}, \tag{1}$$

is called the *j*-sphere of v_i regarding G. $d(v_i, v)$ denotes the shortest distance between the vertices v_i and v.

Definition 2.4. Let $G = (V, E) \in \mathscr{G}_{UC}$. For a vertex $v_i \in V$ we determine the set $S_j(v_i, G) = \{v_{u_j}, v_{v_j}, \ldots, v_{x_j}\}$ and define associated paths:

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

and their edge sets

$$\begin{aligned} E_1 &= \{\{v_i, v_{u_1}\}, \{v_{u_2}, v_{u_3}\}, \ldots, \{v_{u_{j-1}}, v_{u_j}\}\}, \\ E_2 &= \{\{v_i, v_{w_1}\}, \{v_{w_2}, v_{w_3}\}, \ldots, \{v_{w_{j-1}}, v_{w_j}\}\}, \\ &\vdots \\ E_{k_j} &= \{\{v_i, v_{x_1}\}, \{v_{x_2}, v_{x_3}\}, \ldots, \{v_{x_{j-1}}, v_{x_j}\}\}. \end{aligned}$$

Now, we define the graph $\mathscr{L}_G(v_i, j) = (V_{\mathscr{L}}, E_{\mathscr{L}}) \subseteq G$, where

$$V_{\mathscr{L}} := \{v_i, v_{u_1}, v_{u_2}, \ldots, v_{u_j}\} \cup \{v_i, v_{w_1}, v_{w_2}, \ldots, v_{w_j}\} \cup \cdots \cup \{v_i, v_{x_1}, v_{x_2}, \ldots, v_{x_j}\}, \tag{2}$$

and

$$E_{\mathscr{L}} := E_1 \cup E_2 \cup \cdots \cup E_{k_j}. \tag{3}$$

Definition 2.5. Let $G = (V, E) \in \mathscr{G}_{UC}$ and let S initially be an abstract set. Then, we call $f : S \to \mathbb{R}_+$ the information functional of G. We always assume that f is monotonous.

We want to notice that the abstract set S mentioned in Definition 2.5 defines a certain set of associated objects of a graph G, e.g., vertex sets, sets of paths, or certain subgraphs. This set S is used to define the functional f that captures structural information of G. As an example, we show in Fig. 1 the process of determining *j*-spheres for a simple undirected and connected graph G and the derived local information graphs (with respect to a special f, see Definition 2.10).

Definition 2.6. We call $\mathscr{L}_G(v_i, j) = (V_{\mathscr{L}}, E_{\mathscr{L}})$ the local information graph regarding $v_i \in V$ with respect to f. Further,

$$j = j(v_i), \tag{4}$$

is called the local information radius regarding v_i.

As we have already mentioned, the information functional f captures structural information of the underlying graph G and has to be defined concretely. This implies that for defining f arbitrary graph-theoretical properties or quantities can be used. As an important remark, we want to emphasize that the local information graph regarding $v_i \in V$ is not always uniquely defined. This can be understood by the fact that there often exists more than one path from v_i to a certain vertex in the corresponding *j*-sphere. In case we use different information functionals to measure the entropy of a graph, we obviously obtain different probability distributions. Hence, the resulting graph entropies are also different. In Section 3, we present some theoretical results

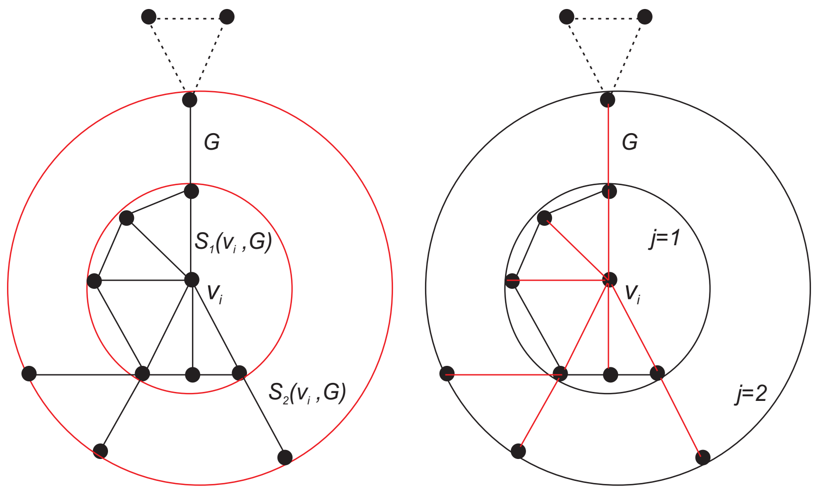

Fig. 1. The left-hand figure shows the determination of j-spheres for a graph $G \in \mathcal{G}_{UC}$ where it holds $|S_1(v_i, G)| = 6$ and $|S_2(v_i, G)| = 4$. The right-hand figure shows the corresponding local information graphs regarding $v_i \in V$ for $j = 1, 2$ with respect to a special information functional f. The local information graphs are depicted by red-colored edges. In this example, f is based on counting certain path lengths (see Definition 2.10). Further, in the right-hand figure, the local information radii for $j = 1, 2$ are depicted. (For interpretation of the references in color in this figure legend, the reader is referred to the web version of this article.)

to investigate relationships between the resulting entropies if different information functionals are used. Starting from the novel definitions, we are now ready to define the entropy of a graph by using an arbitrary information functional.

Definition 2.7. Let $G = (V, E) \in \mathcal{G}_{UC}$ with arbitrary vertex labels. For a vertex $v_i \in V$, we define:

$$p(v_i) := \frac{f(v_i)}{\sum_{j=1}^{|V|} f(v_j)}. \tag{5}$$

f represents an arbitrary information functional. Because it holds the equation:

$$p(v_1) + p(v_2) + \cdots + p(v_{|V|}) = 1,$$

we interpret the quantities $p(v_i)$ as vertex probabilities.

Now, we immediately obtain a definition of a graph entropy of G where this entropy is here interpreted as its mean structural information content.

Definition 2.8. Let $G = (V, E) \in \mathcal{G}_{UC}$ and let f be an arbitrary information functional. We define the entropy of G by

$$I_f(G) := -\sum_{i=1}^{|V|} \frac{f(v_i)}{\sum_{j=1}^{|V|} f(v_j)} \log\left(\frac{f(v_i)}{\sum_{j=1}^{|V|} f(v_j)}\right). \tag{6}$$

2.1. Information functionals: metrical graph properties

In the following, we define two information functionals which are based on metrical properties of graphs. Now, we see that such information functionals can be easily obtained by using the definition of the j-spheres.

Definition 2.9. Let $G = (V, E) \in \mathcal{G}_{UC}$. For a vertex $v_i \in V$, we define the information functional:

$$f^V(v_i) := \alpha^{c_1|S_1(v_i,G)| + c_2|S_2(v_i,G)| + \cdots + c_\rho|S_\rho(v_i,G)|}, \quad c_k > 0, \ 1 \leqslant k \leqslant \rho, \ \alpha > 0, \tag{7}$$

where the c_k are arbitrary real positive coefficients. According to Definition 2.3, $S_j(v_i, G)$ denotes the j-sphere of v_i regarding G and $|S_j(v_i, G)|$ its cardinality, respectively.

The next definition presents a novel information functional f^P where this functional is based on path lengths of the local information graph $\mathscr{L}_G(v_i, j)$ (for each vertex v_i and $j = 1, 2, \ldots, \rho$).

Definition 2.10. Let $G = (V, E) \in \mathscr{G}_{UC}$. For each vertex $v_i \in V$ and for $j = 1, 2, \ldots, \rho$, we determine the local information graph $\mathscr{L}_G(v_i, j)$ where $\mathscr{L}_G(v_i, j)$ is induced by the paths $P_1^j(v_i), P_2^j(v_i), \ldots, P_{k_j}^j(v_i)$. The quantity $l(P_\mu^j(v_i)) \in \mathbb{N},\ \mu \in \{1, 2, \ldots, k_j\}$ denotes the length of $P_\mu^j(v_i)$ and

$$l(P(\mathscr{L}_G(v_i, j))) := \sum_{\mu=1}^{k_j} l(P_\mu^j(v_i)),$$

expresses the sum of the path lengths associated to each $\mathscr{L}_G(v_i, j)$. Now, we define the information functional $f^P(v_i)$ as

$$f^P(v_i) := \alpha^{b_1 l(P(\mathscr{L}_G(v_i,1))) + b_2 l(P(\mathscr{L}_G(v_i,2))) + \cdots + b_\rho l(P(\mathscr{L}_G(v_i,\rho)))}, \quad b_k > 0,\ 1 \leqslant k \leqslant \rho,\ \alpha > 0. \tag{8}$$

b_k are arbitrary real positive coefficients.

Exemplarily, by applying Definitions 2.9 and 2.10, and Eq. (6), we obviously obtain the special entropies

$$I_{f^V}(G) := -\sum_{i=1}^{|V|} \frac{f^V(v_i)}{\sum_{j=1}^{|V|} f^V(v_j)} \log\left(\frac{f^V(v_i)}{\sum_{j=1}^{|V|} f^V(v_j)}\right), \tag{9}$$

and

$$I_{f^P}(G) := -\sum_{i=1}^{|V|} \frac{f^P(v_i)}{\sum_{j=1}^{|V|} f^P(v_j)} \log\left(\frac{f^P(v_i)}{\sum_{j=1}^{|V|} f^P(v_j)}\right). \tag{10}$$

2.2. Information functionals: local property measures

In Section 2.1, we presented information functionals which are based on metrical graph properties, i.e., cardinalities of vertex spheres and path lengths. We want to mention that Definition 2.10 uses the just introduced concept of a local information graph regarding a vertex $v_i \in V$. We now see that this concept gives us the possibility to apply certain graph measures to the obtained local information graphs for defining novel information functionals and, hence, novel graph entropy measures. In the following, we define an information functional by using so called *local property measures*. By a local property measure, we understand a graph measure that characterizes graph elements (e.g., vertices of a graph) regarding a local structural property, e.g., the *centrality* of a vertex [1,2,4,19,30,34]. For example, if we consider the centrality concept based on shortest paths in a graph, then such a vertex centrality measure $\beta(v_i),\ v_i \in V$ indicates that v_i can reach other vertices on relatively short paths [4]. Starting from a vertex $v_i \in V$, this finally means that an information functional based on a certain local property measure quantifies structural information of a graph concerning the chosen property, e.g., closeness or degree centrality [4,30,34]. One prominent example for such a measure that is well-known in the theory of social networks is given by [4,34]

$$\beta(v) = \frac{1}{\sum_{i=1}^{|V|} d(v, v_i)}. \tag{11}$$

To apply this measure exemplarily, we consider Fig. 2 and see the local information graphs $\mathscr{L}_G(v_i, 1)$ and $\mathscr{L}_G(v_i, 2)$ of G depicted in Fig. 1. Then, the computation of the vertex centrality measure β regarding v_i leads to

$$\beta^{\mathscr{L}_G(v_i,1)}(v_i) = \frac{1}{1+1+1+1+1+1} = \frac{1}{6},$$

and

$$\beta^{\mathscr{L}_G(v_i,2)}(v_i) = \frac{1}{3+3+3+3+2+3+2} = \frac{1}{11}.$$

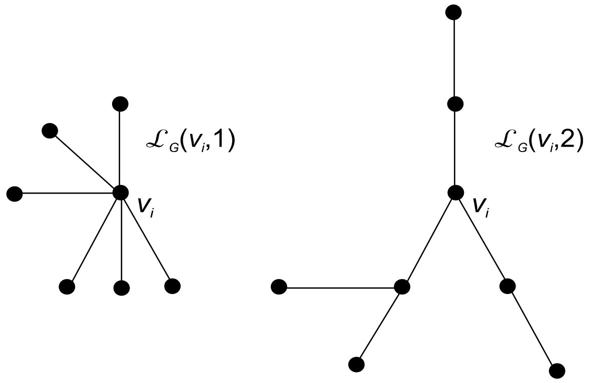

Fig. 2. The local information graphs $\mathscr{L}_G(v_i,1)$ and $\mathscr{L}_G(v_i,2)$ of G shown in Fig. 1.

In order to avoid confusion with the above notation, we remark that $\beta^{\mathscr{L}_G(v_i,j)}(v_i)$ expresses that we apply β to v_i regarding $\mathscr{L}_G(v_i,j)$. Now, we are ready to define a novel information functional f^C that is based on a vertex centrality measure.

Definition 2.11. Let $G=(V,E)\in\mathscr{G}_{UC}$ and $\mathscr{L}_G(v_i,j)$ denotes the local information graph (see Definition 2.6) for each vertex $v_i\in V$. We define $f^C(v_i)$ as

$$f^C(v_i):=\alpha^{a_1\beta^{\mathscr{L}_G(v_i,1)}(v_i)+a_2\beta^{\mathscr{L}_G(v_i,2)}(v_i)+\cdots+a_\rho\beta^{\mathscr{L}_G(v_i,\rho)}(v_i)},\quad \beta\leqslant 1,\ a_k>0,\ 1\leqslant k\leqslant\rho,\ \alpha>0, \tag{12}$$

where β is a certain vertex centrality measure and a_k are arbitrary real positive coefficients.

2.3. Complexity analysis

For finalizing Section 2, we analyze the computational complexity of our resulting entropy measure $I_f(G)$ if we use the presented information functionals $f^V,\ f^P$ and f^C. We first notice that the computation of $f^V,\ f^P$ and f^C depends on determining j-spheres, for all vertices $v_i\in V$ in a graph $G=(V,E)\in\mathscr{G}_{UC}$ with an associated weight function $\omega:E\rightarrow\{1\}$. That is, we have to compute the distances $d(v_i,v_j)$, for all pairs $v_i,v_j\in V$. But to compute those distances, we can apply an existing shortest path algorithm, e.g., Dijkstra's algorithm [11] $|V|$ times for each vertex as a starting point. It was proven [8] that this algorithm requires time complexity $O(|V|^3)$. Particularly, we observe that the time complexity for computing the quantities $p^V(v_i),\ p^P(v_i)$ and $p^C(v_i)$ is $O(|V|^2)$ because we have to parse the adjacency matrix of G starting from v_i. Based on these considerations, we finally obtain the following assertion.

Theorem 2.1. *The time complexity to compute the entropies $I_{f^V}(G),\ I_{f^P}(G)$, and $I_{f^C}(G)$ for $G\in\mathscr{G}_{UC}$ is $O(|V|^3)$.*

3. Relations for graph entropies

The main goal of this section is to investigate relationships between the resulting graph entropies represented by inequalities. Because we are now able to use arbitrary information functionals to finally quantify the structural information content of networks, we need assertions for examining the influence of an information functional under consideration. In the following, we first explore the relatedness between the previously defined functionals of Section 2.1 and finally of the associated entropies. For this, we first state a technical assertion as follows.

Proposition 3.1. *Let $G=(V,E)\in\mathscr{G}_{UC}$. For each vertex $v_i\in V$ and for the information radii $j=1,2,\ldots,\rho$, it holds*

$$l(P(\mathscr{L}_G(v_i,j)))=j\cdot|S_j(v_i,G)|. \tag{13}$$

Proof. Let $v_i \in V$ and let $S_j(v_i, G)$ the j-sphere where its number of vertices is denoted by $|S_j(v_i, G)|$. Based on the definition of the local information graph regarding v_i, there exist exactly $|S_j(v_i, G)|$ paths with length j. This leads directly to the equation $l(P(\mathscr{L}_G(v_i, j))) = j \cdot |S_j(v_i, G)|$. $\square$

Based on Proposition 3.1, we now able to express a relationship between the vertex probability values regarding the information functionals f^V and f^P.

Theorem 3.2. *Let $G = (V, E) \in \mathscr{G}_{UC}$ and let f^V and f^P be the defined information functionals. If we define*

$$\omega^P(v_i) := \max_{1 \leqslant j \leqslant \rho} l(P(\mathscr{L}_G(v_i, j))), \quad \omega^P := \max_{1 \leqslant i \leqslant |V|} \omega^P(v_i), \quad \phi^P := \max_{1 \leqslant j \leqslant \rho} b_j \quad \textit{and} \quad \varphi := \min_{1 \leqslant j \leqslant \rho} c_j,$$

then, the inequality

$$p^V(v_i) < \alpha^{\rho[\phi^P \omega^P - \varphi]} \cdot p^P(v_i), \quad \rho[\phi^P \omega^P - \varphi] > 0, \ \alpha > 1, \tag{14}$$

holds. $p^V(v_i)$ and $p^P(v_i)$ denotes the i-th vertex probability regarding f^V and f^P.

Proof. Let $G = (V, E) \in \mathscr{G}_{UC}$. Based on the definition of f^V and f^P and the assumption that $c_i \leqslant b_i$, we get with Proposition 3.1

$$f^V(v_i) = \alpha^{c_1|S_1(v_i,G)|+c_2|S_2(v_i,G)|+\cdots+c_\rho|S_\rho(v_i,G)|} \leqslant \alpha^{b_1 l(P(\mathscr{L}_G(v_i,1)))+b_2 l(P(\mathscr{L}_G(v_i,2)))+\cdots+b_\rho l(P(\mathscr{L}_G(v_i,\rho)))} = f^P(v_i),$$

if $\alpha > 1$. Now, starting from the inequality $f^V(v_i) \leqslant f^P(v_i)$, we further obtain:

$$\begin{aligned} p^V(v_i) &= \frac{\alpha^{c_1|S_1(v_i,G)|+c_2|S_2(v_i,G)|+\cdots+c_\rho|S_\rho(v_i,G)|}}{\sum_{j=1}^{|V|} f^V(v_j)} \leqslant \frac{\alpha^{b_1 l(P(\mathscr{L}_G(v_i,1)))+b_2 l(P(\mathscr{L}_G(v_i,2)))+\cdots+b_\rho l(P(\mathscr{L}_G(v_i,\rho)))}}{\sum_{j=1}^{|V|} f^V(v_j)} \\ &\leqslant \frac{\alpha^{b_1 l(P(\mathscr{L}_G(v_i,1)))+b_2 l(P(\mathscr{L}_G(v_i,2)))+\cdots+b_\rho l(P(\mathscr{L}_G(v_i,\rho)))}}{\sum_{j=1}^{|V|} f^P(v_j)} \cdot \frac{\sum_{j=1}^{|V|} f^P(v_j)}{\sum_{j=1}^{|V|} f^V(v_j)} = p^P(v_i) \cdot \frac{\sum_{j=1}^{|V|} f^P(v_j)}{\sum_{j=1}^{|V|} f^V(v_j)}. \end{aligned} \tag{15}$$

By using the definition of $\omega^P(v_i)$, ω^P, ϕ^P and φ, it holds

$$\begin{aligned} f^P(v_i) &= \alpha^{b_1 l(P(\mathscr{L}_G(v_i,1)))+b_2 l(P(\mathscr{L}_G(v_i,2)))+\cdots+b_\rho l(P(\mathscr{L}_G(v_i,\rho)))} \leqslant \alpha^{b_1\omega^P(v_i)+b_2\omega^P(v_i)+\cdots+b_\rho\omega^P(v_i)} < \alpha^{\phi^P\omega^P(v_i)+\phi^P\omega^P(v_i)+\cdots+\phi^P\omega^P(v_i)} \\ &= \alpha^{\rho\cdot\phi^P\cdot\omega^P(v_i)}, \end{aligned}$$

and, hence,

$$\sum_{j=1}^{|V|} f^P(v_j) < |V| \alpha^{\rho\cdot\phi^P\cdot\omega^P}. \tag{16}$$

Similarly, we have:

$$f^V(v_i) = \alpha^{c_1|S_1(v_i,G)|+c_2|S_2(v_i,G)|+\cdots+c_\rho|S_\rho(v_i,G)|} > \alpha^{c_1+c_2+\cdots+c_\rho} > \alpha^{\rho\cdot\varphi},$$

and

$$\sum_{j=1}^{|V|} f(v_j) > |V| \alpha^{\rho\cdot\varphi}. \tag{17}$$

By applying inequality (16) and (17), inequality (15) finally becomes to

$$p^V(v_i) < p^P(v_i) \cdot \frac{|V|\alpha^{\rho\cdot\phi^P\cdot\omega^P}}{|V|\alpha^{\rho\cdot\varphi}} = p^P(v_i) \cdot \alpha^{\rho[\phi^P\omega^P - \varphi]}.$$

But this inequality equals inequality (14), the assertion of the theorem. $\square$

Now, we use the result of Theorem 3.2 to express a relationship between the resulting graph entropies.

Theorem 3.3. *Let $G = (V, E) \in \mathcal{G}_{UC}$ and let f^V and f^P be the defined information functionals. For the associated graph entropies, it holds the inequality*:

$$I_{f^V}(G) > \alpha^{\rho[\phi^P \omega^P - \varphi]}\left[I_{f^P}(G) - \log\left(\alpha^{\rho[\phi^P \omega^P - \varphi]}\right)\right], \quad \alpha > 1. \tag{18}$$

Proof. We start with considering inequality (14). If we multiply this inequality by -1, we get:

$$-p^V(v_i) > -\alpha^{\rho[\phi^P \omega^P - \varphi]} \cdot p^P(v_i). \tag{19}$$

Now, by using the assertion of Theorem 3.2 and the monotonicity property of the logarithm function, we first obtain:

$$-p^V(v_i)\log(p^V(v_i)) > -\alpha^{\rho[\phi^P \omega^P - \varphi]} \cdot p^P(v_i) \cdot \log(p^P(v_i)) - \alpha^{\rho[\phi^P \omega^P - \varphi]} \cdot p^P(v_i) \cdot \log\left(\alpha^{\rho[\phi^P \omega^P - \varphi]}\right). \tag{20}$$

By doing this step for each vertex $v_i \in V$ and by adding the obtained inequalities, one gets:

$$\begin{aligned} &-p^V(v_1)\log(p^V(v_1)) - p^V(v_2)\log(p^V(v_2)) - \cdots - p^V(v_{|V|})\log(p^V(v_{|V|})) \\ &\quad > \alpha^{\rho[\phi^P \omega^P - \varphi]}\left[-p^P(v_1)\log(p^P(v_1)) - p^P(v_2)\log(p^P(v_2)) - \cdots - p^P(v_{|V|})\log(p^P(v_{|V|}))\right] - \alpha^{\rho[\phi^P \omega^P - \varphi]} \\ &\quad \times \log\left(\alpha^{\rho[\phi^P \omega^P - \varphi]}\right)\sum_{j=1}^{|V|} p^P(v_j) \\ &\quad = \alpha^{\rho[\phi^P \omega^P - \varphi]}\left[-p^P(v_1)\log(p^P(v_1)) - p^P(v_2)\log(p^P(v_2)) - \cdots - p^P(v_{|V|})\log(p^P(v_{|V|}))\right] - \alpha^{\rho[\phi^P \omega^P - \varphi]} \\ &\quad \times \log\left(\alpha^{\rho[\phi^P \omega^P - \varphi]}\right). \end{aligned}$$

That is, it holds:

$$\begin{aligned} &-p^V(v_1)\log(p^V(v_1)) - p^V(v_2)\log(p^V(v_2)) - \cdots - p^V(v_{|V|})\log(p^V(v_{|V|})) \\ &\quad > \alpha^{\rho[\phi^P \omega^P - \varphi]}\left[-p^P(v_1)\log(p^P(v_1)) - p^P(v_2)\log(p^P(v_2)) - \cdots - p^P(v_{|V|})\log(p^P(v_{|V|}))\right] - \alpha^{\rho[\phi^P \omega^P - \varphi]} \\ &\quad \times \log\left(\alpha^{\rho[\phi^P \omega^P - \varphi]}\right). \end{aligned} \tag{21}$$

By using the definition of the graph entropy, inequality (21) becomes finally to

$$I_{f^V}(G) > \alpha^{\rho[\phi^P \omega^P - \varphi]}\left[I_{f^P}(G) - \log\left(\alpha^{\rho[\phi^P \omega^P - \varphi]}\right)\right],$$

thus, inequality (18). □

In order to express a relation for the vertex probabilities regarding f^V and f^C, we use same principle as shown in the proof of Theorem 3.2 and obtain the following theorem.

Theorem 3.4. *Let $G = (V, E) \in \mathcal{G}_{UC}$ and let f^V and f^C be the defined information functionals. For the vertex probabilities $p^V(v_i)$ and $p^C(v_i)$, it holds*:

$$p^V(v_i) > \alpha^{\rho[\varphi^C m^C - \phi \cdot \omega]} \cdot p^C(v_i), \quad c_i \geqslant a_i, \; \alpha > 1, \tag{22}$$

where $\omega(v_i) := \max_{1 \leqslant j \leqslant \rho}|S_j(v_i, G)|$, $\omega := \max_{1 \leqslant i \leqslant |V|}(\omega(v_i))$, $\phi := \max_{1 \leqslant j \leqslant \rho} c_j$, $\varphi^C := \min_{1 \leqslant j \leqslant \rho} a_j$, *and* $m^C := \min_{1 \leqslant i \leqslant |V|} m^C(v_i)$.

Now, we straightforward express a theorem that gives us a relationship for the associated graph entropies of f^V and f^C.

Theorem 3.5. *Let $G = (V, E) \in \mathcal{G}_{UC}$ and let f^V and f^C be the defined information functionals. For the associated graph entropies, it holds the relation*:

$$I_{f^V}(G) < \alpha^{\rho[\varphi^C m^C - \phi \cdot \omega]}\left[I_{f^C}(G) - \log\left(\alpha^{\rho[\varphi^C m^C - \phi \cdot \omega]}\right)\right], \quad \alpha > 1. \tag{23}$$

Proof. By using the assertion of Theorem 3.4, the proof of Theorem 3.5 can be obtained by analogously applying the technique and steps of the proof of Theorem 3.3. □

As a final remark for this section, we note that one can easily obtain similar assertions for the relationship between the vertex probabilities and the associated graph entropies regarding f^P and f^C.

4. Numerical results

In the following, we numerically determine the entropies of the example graphs of Fig. 3 by using the information functionals f^V, f^P and f^C. Based on the obtained numerical results, we are able to compare the resulting graph entropies to study the influence of the chosen information functionals. To obtain the numerical results for our example graphs G_1 and G_2, we now apply Definitions 2.9 and 2.10 and Proposition 3.1. As an important remark, we notice that we generally choose the coefficients $c_k,\ b_k$ and a_k for emphasizing certain structural characteristics of the underlying graphs, e.g., high vertex degrees etc. Without loss of generality, we now choose the $c_k,\ b_k$ and a_k such that $c_k = b_k = a_k$ and $c_1 > c_2 > c_3 > c_4$. Here, we set $c_1 := 4,\ c_2 := 3,\ c_3 := 2,\ c_4 = 1$. Further, we observe that for G_1 it holds $\rho(G_1) = 4$. Now, by applying Definition 2.9, we obtain:

$$f^V(v_1) = f^V(v_4) = f^V(v_5) = f^V(v_8) = \alpha^{2c_1+2c_2+2c_3+c_4}, \tag{24}$$

$$f^V(v_2) = f^V(v_7) = \alpha^{2c_1+3c_2+2c_3}, \tag{25}$$

$$f^V(v_3) = f^V(v_6) = \alpha^{3c_1+3c_2+c_3}. \tag{26}$$

By using the defined values for c_k, we get:

$$f^V(v_1) = f^V(v_4) = f^V(v_5) = f^V(v_8) = \alpha^{19}, \tag{27}$$

$$f^V(v_2) = f^V(v_7) = \alpha^{21}, \tag{28}$$

$$f^V(v_3) = f^V(v_6) = \alpha^{23}. \tag{29}$$

Now, if we now apply Eq. (5) and Definition 2.8, the equation to express the structural information content of G_1 becomes to

$$\begin{aligned} I_{f^V}(G_1) &:= -\sum_{i=1}^{8} p^V(v_i)\log(p^V(v_i)) = -\left[4\frac{\alpha^{19}}{4\alpha^{19}+2\alpha^{21}+2\alpha^{23}}\log\left(\frac{\alpha^{19}}{4\alpha^{19}+2\alpha^{21}+2\alpha^{23}}\right)\right. \\ &\left. +2\frac{\alpha^{21}}{4\alpha^{19}+2\alpha^{21}+2\alpha^{23}}\log\left(\frac{\alpha^{21}}{4\alpha^{19}+2\alpha^{21}+2\alpha^{23}}\right)+2\frac{\alpha^{23}}{4\alpha^{19}+2\alpha^{21}+2\alpha^{23}}\log\left(\frac{\alpha^{23}}{4\alpha^{19}+2\alpha^{21}+2\alpha^{23}}\right)\right]. \end{aligned} \tag{30}$$

To compute the entropy of G_1 regarding f^P, we straightforward apply Proposition 3.1 to the Eqs. (24)–(26), and infer

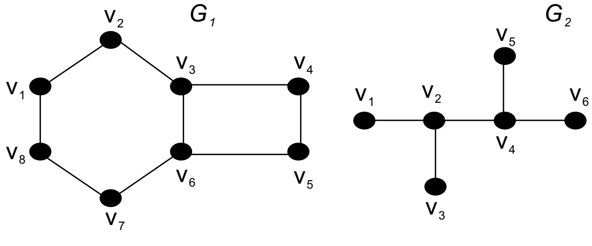

Fig. 3. G_1 and G_2 are undirected and connected graphs.

$$f^P(v_1) = f^P(v_4) = f^P(v_5) = f^P(v_8) = \alpha^{2c_1+4c_2+6c_3+4c_4}, \tag{31}$$
$$f^P(v_2) = f^P(v_7) = \alpha^{2c_1+6c_2+6c_3}, \tag{32}$$
$$f^P(v_3) = f^P(v_6) = \alpha^{3c_1+6c_2+3c_3}, \tag{33}$$
$$f^P(v_1) = f^P(v_4) = f^P(v_5) = f^P(v_8) = \alpha^{36}, \tag{34}$$
$$f^P(v_2) = f^P(v_3) = f^P(v_6) = f^P(v_7) = \alpha^{38}, \tag{35}$$

and, hence,

$$\begin{aligned} I_{f^P}(G_1) &:= -\sum_{i=1}^{8} p^P(v_i)\log(p^P(v_i)), \\ &= -\left[6\frac{\alpha^{36}}{6\alpha^{36}+2\alpha^{38}}\log\left(\frac{\alpha^{36}}{6\alpha^{36}+2\alpha^{38}}\right) + 2\frac{\alpha^{38}}{6\alpha^{36}+2\alpha^{38}}\log\left(\frac{\alpha^{38}}{6\alpha^{36}+2\alpha^{38}}\right)\right]. \end{aligned} \tag{36}$$

In order to compute I_{f^C} for G_1, we exemplarily use Eq. (11) as local property measure. Eq. (11) expresses how central a vertex v_i of the local information graph $\mathscr{L}_G(v_i, j)$ is. Once again, we want to emphasize that the local information graph can be sometimes not uniquely obtained because there often exists more than one path from v_i to a certain vertex in the corresponding j-sphere. In such a case, we therefore choose $\mathscr{L}_G(v_i, j)$ such that $\beta^{\mathscr{L}_G(v_i,j)}(v_i)$ attains its maximum. Starting from this assumption, we have:

$$f^C(v_1) = f^C(v_8) = \alpha^{2.82}, \tag{37}$$
$$f^C(v_4) = f^C(v_5) = \alpha^{2.88}, \tag{38}$$
$$f^C(v_2) = f^C(v_7) = \alpha^{2.59}, \tag{39}$$
$$f^C(v_3) = \alpha^{2.08}, \tag{40}$$
$$f^C(v_6) = \alpha^{2.04}, \tag{41}$$

and

$$\begin{aligned} I_{f^C}(G_1) := -\sum_{i=1}^{8} p^C(v_i)\log(p^C(v_i)) = -\Bigg[&2\frac{\alpha^{2.82}}{\sum_{j=8} f^C(v_j)}\log\left(\frac{\alpha^{2.82}}{\sum_{j=8} f^C(v_j)}\right) \\ &+2\frac{\alpha^{2.88}}{\sum_{j=8} f^C(v_j)}\log\left(\frac{\alpha^{2.88}}{\sum_{j=8} f^C(v_j)}\right) + 2\frac{\alpha^{2.59}}{\sum_{j=8} f^C(v_j)}\log\left(\frac{\alpha^{2.59}}{\sum_{j=8} f^C(v_j)}\right) \\ &+\frac{\alpha^{2.08}}{\sum_{j=8} f^C(v_j)}\log\left(\frac{\alpha^{2.08}}{\sum_{j=8} f^C(v_j)}\right) + \frac{\alpha^{2.04}}{\sum_{j=8} f^C(v_j)}\log\left(\frac{\alpha^{2.04}}{\sum_{j=8} f^C(v_j)}\right)\Bigg], \end{aligned} \tag{42}$$

where $\sum_{j=8} f^C(v_j) = 2\alpha^{2.82} + 2\alpha^{2.88} + 2\alpha^{2.59} + \alpha^{2.08} + \alpha^{2.04}$. By applying the same steps as stated above, the process of determining the structural information content of $I_{f^V}(G_2)$, $I_{f^P}(G_2)$ and $I_{f^C}(G_2)$ (it holds $\rho(G_2) = 3$) is the same. Finally, we obtain:

$$\begin{aligned} I_{f^V}(G_2) &:= -\sum_{i=1}^{6} p^V(v_i)\log(p^V(v_i)) \\ &= -\left[4\frac{\alpha^{14}}{4\alpha^{14}+2\alpha^{18}}\log\left(\frac{\alpha^{14}}{4\alpha^{14}+2\alpha^{18}}\right) + 2\frac{\alpha^{18}}{4\alpha^{14}+2\alpha^{18}}\log\left(\frac{\alpha^{18}}{4\alpha^{14}+2\alpha^{18}}\right)\right], \end{aligned} \tag{43}$$

$$\begin{aligned} I_{f^P}(G_2) &:= -\sum_{i=1}^{6} p^P(v_i)\log(p^P(v_i)) \\ &= -\left[4\frac{\alpha^{28}}{4\alpha^{28}+2\alpha^{24}}\log\left(\frac{\alpha^{28}}{4\alpha^{28}+2\alpha^{24}}\right) + 2\frac{\alpha^{24}}{4\alpha^{28}+2\alpha^{24}}\log\left(\frac{\alpha^{24}}{4\alpha^{28}+2\alpha^{24}}\right)\right], \end{aligned} \tag{44}$$

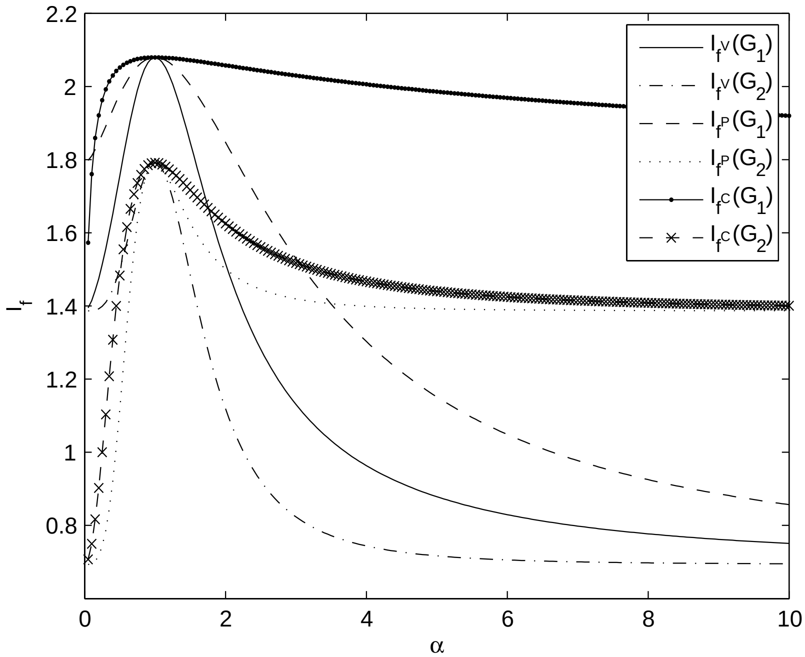

Fig. 4. Entropies of the graphs G_1 and G_2 shown in Fig. 3 regarding the information functionals f^V, f^P and f^C. The entropies are plotted in dependence of the value α.

and

$$I_{f^C}(G_2) := -\sum_{i=1}^{6} p^C(v_i)\log(p^C(v_i))$$
$$= -\left[4\frac{\alpha^{4.28}}{4\alpha^{4.28}+2\alpha^{1.93}}\log\left(\frac{\alpha^{4.28}}{4\alpha^{4.28}+2\alpha^{1.93}}\right)+2\frac{\alpha^{1.93}}{4\alpha^{4.28}+2\alpha^{1.93}}\log\left(\frac{\alpha^{1.93}}{4\alpha^{4.28}+2\alpha^{1.93}}\right)\right]. \quad (45)$$

Now, to interpret the numerical results we look at Fig. 4. We first consider the entropies of G_1 and G_2 regarding the information functionals f^V and f^P. Here, the entropies were plotted in dependence of the free parameter α. As a first result, we observe that the graph entropy $I_{f^V}(G_1)$ is always larger than $I_{f^V}(G_2)$. In terms of the interconnectedness, this can be explained by the intuitive observation that G_1 is structurally more complex than the graph structure of G_2. We also see that based on the definition of f^V, a stronger branching of a graph leads to larger values of the cardinalities of the j-spheres. In case of using the information functional f^P, we also see in Fig. 4 that $I_{f^P}(G_1)$ is always larger than $I_{f^P}(G_2)$. This observation can be easily understood by applying Proposition 3.1. The assertion of this proposition is that the sum of the path lengths of the local information graph regarding a vertex v_i is equal to the product of the cardinality of the corresponding j-sphere and the value of the local information radius. If $\alpha > 1$, this implies that the sum of the exponents of f^P is always larger than in case of f^V. For interpreting the numerical results regarding the information functional f^C, we observe that it holds $I_{f^C}(G_1) > I_{f^C}(G_2)$. This result corresponds with the observations achieved in case of using f^V and f^P. In this case we also find that for $\alpha > 1$, the values of the entropies $I_{f^C}(G_1)$ and $I_{f^C}(G_2)$ are always larger than the values of the other corresponding graph entropies. Starting from the defined information functionals we finally find that our entropy measure is able to reflect the essence of graph branching meaningfully.

5. Summary and conclusion

This paper dealt with the problem of analyzing and understanding information processing in complex networks by using information-theoretical methods. One major problem we addressed was to quantify structural information in networks based on so called information functionals. In this work we considered a complex network as an undirected and connected graph. Based on such information functionals, different graphs entropies can be directly defined. As a generalization, we introduced the definition of the local information graph and of the local information radius. Starting from these definitions, we are now able to define the entropy of a graph by using several structural properties or local property measures. As examples for information functionals, we used functionals which are based on metrical properties of graphs, e.g., vertex spheres, path lengths and local property measures (shortest path centrality) for finally investigating the behavior of the resulting graph entropy. Then, in Section 2, we further noticed that the computational complexity to determine the final graph entropies is polynomial. As a main result of this paper, we proved theorems for describing relationships between graph entropies concerning the defined information functionals. This is an important step to obtain theoretical results for comparing graph entropies and for studying the influence of the information functionals under consideration. The obtained inequalities can be also very useful to classify graphs regarding their entropies. Finally, in Section 4, we presented some numerical results to study the influence of the different information functionals on the resulting entropies. We obtained the result that the entropy measures based on the defined information functionals (f^V, f^P, and I^C) can detect the structural complexity between graphs and therefore capture important structural information meaningfully.

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References

[1] A. Bavelas, A mathematical model for group structure, Hum. Organ. 7 (1948) 16–30.
[2] A. Bavelas, Communication patterns in task-oriented groups, J. Acoust. Soc. Am. 22 (1950) 725–730.
[3] D. Bonchev, Information Theoretic Indices for Characterization of Chemical Structures, Research Studies Press, Chichester, 1983.
[4] U. Brandes, A faster algorithm for betweenness centrality, J. Math. Sociol. 25 (2) (2001) 163–177.
[5] F. Buckley, F. Harary, Distance in Graphs, Addison Wesley Publishing Company, 1990.
[6] J.C. Claussen, Characterization of networks by the offdiagonal complexity, Physica A 365–373 (2007) 321–354.
[7] J.C. Claussen, Offdiagonal complexity: a computationally quick network complexity measure – application to protein networks and cell division, in: A. Deutsch, R. Bravo de la Parra, R. de Boer, O. Diekmann, P. Jagers, E. Kisdi, M. Kretzschmar, P. Lansky, H. Metz (Eds.), Mathematical Modeling of Biological Systems, vol. II, Birkhäuser, Boston, 2007, pp. 303–311.
[8] T.H. Cormen, C.E. Leiserson, R.L. Rivest, Introduction to Algorithms, MIT Press, 1990.
[9] M. Dehmer, A novel method for measuring the structural information content of networks, Cybern. Syst. (2007) in press.
[10] M. Dehmer, F. Emmert-Streib, Local information spread in networks, Private Communication, Seattle, USA, 2007.
[11] E.W. Dijkstra, A note on two problems in connection with graphs, Numer. Math. 1 (1959) 269–271.
[12] M.V. Diudea, I. Gutman, L. Jäntschi, Molecular Topology, Nova Publishing, 2001.
[13] F. Emmert-Streib, The chronic fatigue syndrome: a comparative pathway analysis, J. Comput. Biol. 14 (7) (2007).
[14] F. Emmert-Streib, M. Dehmer, Information theoretic measures of UHG graphs with low computational complexity, Appl. Math. Comput. 190 (2) (2007) 1783–1794.
[15] F. Emmert-Streib, M. Dehmer, Global information processing in gene networks: fault tolerance, in: Proceedings of the Workshop on Computing and Communications from Biological Systems: Theory and Applications, in press.
[16] A.L. Fradkov, Cybernetical Physics: From Control of Chaos to Quantum Control, Springer, 2007.
[17] C. Godsil, G. Royle, Algebraic Graph Theory. Graduate Texts in Mathematics, Academic Press, 2001.
[18] I. Gutman, O.E. Polansky, Mathematical Concepts in Organic Chemistry, Springer, 1986.
[19] F. Harary, Structural Models. An Introduction to the Theory of Directed Graphs, Wiley, 1965.
[20] F. Harary, Graph Theory, Addison Wesley Publishing Company, 1969.
[21] J. Koerner, Coding of an information source having ambiguous alphabet and the entropy of graphs, in: Transactions of the Sixth Prague Conference on Information Theory, 1973, pp. 411–425.
[22] T.R. Lezon, J.R. Banavar, M. Cieplak, A. Maritan, N.V. Fedoroff, Using the principle of entropy maximization to infer genetic interaction networks from gene expression patterns, Proc. Natl. Acad. Sci. 103 (50) (2006) 19033–19038.
[23] G.F. Luger, Artificial Intelligence: Structures and Strategies for Complex Problem Solving, Addison Wesley, 2004.
[24] A. Mowshowitz, Entropy and the complexity of graphs. II: The information content of digraphs and infinite graphs, Bull. Math. Biophys. 30 (1968) 225–240.
[25] A. Mowshowitz, Entropy and the complexity of graphs. III: Graphs with prescribed information content, Bull. Math. Biophys. 30 (1968) 387–414.

[26] A. Mowshowitz, Entropy and the complexity of graphs. IV: Entropy measures and graphical structure, Bull. Math. Biophys. 30 (1968) 533–546.
[27] A. Mowshowitz, Entropy and the complexity of the graphs. I: An index of the relative complexity of a graph, Bull. Math. Biophys. 30 (1968) 175–204.
[28] C.V. Negotia, Cybernetics and Applied Systems, CRC Press, 1992.
[29] N. Rashewsky, Life, information theory, and topology, Bull. Math. Biophys. 17 (1955) 229–235.
[30] F. Scott, Social Network Analysis, Sage Publications, 2001.
[31] V.A. Skorobogatov, A.A. Dobrynin, Metrical analysis of graphs, MATCH 23 (1988) 105–155.
[32] N. Trinajstivć, Chemical Graph Theory, CRC Press, 1992.
[33] E. Trucco, A note on the information content of graphs, Bull. Math. Biol. 18 (2) (1956) 129–135.
[34] S. Wasserman, K. Faust, Social network analysis: methods and applications, Structural Analysis in the Social Sciences, Cambridge University Press, 1994.
[35] W.H. Zurek, Complexity, Entropy and the Physics of Information, Westview Press, 1990.