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INFORMATION-THEORETIC CONCEPTS FOR THE ANALYSIS OF COMPLEX NETWORKS

Matthias Dehmer
Vienna University of Technology, Vienna, Austria

□ *In this article, we present information-theoretic concepts for analyzing complex networks. We see that the application of information-theoretic concepts to networks leads to interesting tasks and gives a possibility for understanding information processing in networks. The main contribution of this article is a method for determining the structural information content of graphs that is based on a tree decomposition. It turns out that the computational complexity of the underlying algorithm is polynomial. Finally, we present some numerical results to study the influence of the used methods on the resulting information contents.*

INTRODUCTION

In many scientific areas, e.g., biology, chemistry, linguistics, and physics, it is known that systems can be described as interaction networks of the underlying components (Bonchev and Rouvray 2005; Mehler 2006). Such networks, e.g., protein-protein, signaling, synthesis, and reaction networks, have been intensely investigated, especially in computer science, computational biology, and chemistry (Bonchev and Rouvray 2005; Claussen 2007b; Emmert-Streib 2007; Gagneur, Krause, Bouwmeester, and Casari 2004; Temkin, Zeigarnik, and Bonchev 1996). Once a network is theoretically or experimentally inferred, existing methods from quantitative network analysis are basically applicable for investigating such networks structurally. The two main categories in this area deal with network comparison and characterization, respectively. The problem of structurally comparing networks is mostly understood as the task of measuring their structural similarity. This task is often referred to as graph matching (Bunke 1983; Bunke 2000a,b,

Address correspondence to Matthias Dehmer, Institute of Discrete Mathematics and Geometry, Vienna University of Technology, Wiedner Hauptstrasse 8–10, 1040 Vienna, Austria. E-mail: mdehmer@geometrie.tuwien.ac.at

1998; Bunke and Neuhaus 2007; Dehmer and Mehler 2007; Emmert-Streib, Dehmer, and Kilian 2005; Gernert 1979; Kaden 1982, 1986; Sobik 1982, 1986; Solé and Valverde 2004; Zelinka 1975). In contrast, to characterize networks structurally means that we are searching for so-called network characteristics (Barabasi and Oltvai 2004; Bornholdt and Schuster 2003; Brandes and Erlebach 2005; Gaertler 2005; Dorogovtsev and Mendes 2003; Mason and Verwoerd 2007; Skorobogatov and Dobrynin 1988) which capture structural information of the given networks.

Another paradigm for analyzing complex networks can be obtained by combining methods from graph theory, information theory, and statistics. Particularly, it turned out that information-theoretic methods, e.g., entropy-based approaches are powerful tools to investigate complex systems on a graph or sequence-based level (Bonchev and Rouvray 2005; Bonchev 1983; Claussen 2007a; Kullback 1959; Kullback and Leibler 1951; Shannon and Weaver 1997; Solé and Valverde 2004). In order to give a short overview on such methods, we now briefly outline the most important information-theoretic and statistical methods to characterize or compare network structures:

- Classical information measures, e.g., entropy, conditional entropy, andmutual information applied to complex networks (Bonchev 1979, 1983, 2003; Bonchev, Balaban, and Mekenyan 1980; Bonchev and Trinajstić 1977; Bonchev and Rouvray 2005; Fujii and Yuki 1997; Kieffer and Yang 1997; Shannon and Weaver 1997; Solé and Valverde 2004).
- Entropic measures for characterizing graph classes, e.g., perfect graphs (Körner 1973; Simonyi 2001).
- Information-theoretic measures to determine the structural information content of a network (Bonchev 1983; Dehmer 2007b; Dehmer and Emmert-Streib 2008; Mowshowitz 1968a–d; Rashewsky 1955; Trucco 1956).
- Complexity measures for networks based on the principle of Kolmogorov-complexity (Bonchev 1995, 2003; Li and Vitányi 1997).
- Information-theoretic robustness measures for complex networks (Emmert-Streib and Dehmer 2008a, 2007c).
- Statistical correlation measures for structurally characterizing complex networks (Solé and Valverde 2004).
- Simulated annealing methods to investigate network structures (Solé and Valverde 2004; Schweitzer, Ebeling, Rosé, and Weiss 1996).

In this article, we mainly deal with the problem of applying SHANNON's theory (Shannon and Weaver 1997) to complex network structures. Here, a structure is considered as an outcome of an arbitrary communication

(Bonchev 2003). Then, the classical SHANNON-entropy can be used to determine the so-called structural information content of a network (Mowshowitz 1968–d; Rashewsky 1955; Trucco 1956) where this information content will be interpreted as the entropy of the underlying network topology. A main focus of this article is to develop methods to determine the structural information content of graphs which are efficiently computable, i.e., the time complexity of the underlying algorithm is polynomial. As a short outline, the main contribution of this article is a method for determining the structural information content of graphs by using a graph decomposition approach. For this, we also introduce some special information functionals that quantify structural information of a decomposed graph. We remark that a method to determine the structural information content of arbitrary graphs by using an information functional approach has been introduced in Dehmer (2007b). The computational complexity of the decomposition approach will be analyzed in the section entitled Complexity Analysis. Other concepts we want to present, i.e., local information graphs and further information functionals have already been introduced in Dehmer (2008a).

STRUCTURAL INFORMATION CONTENT OF GRAPHS

We begin by stating some application areas dealing with information-theoretic concepts applied to networks. More precisely, we want to focus on such applications that address the problem of quantifying structural information in networks. In order to give a short overview on the existing methods, we outline some known approaches for determining the structural information content of graphs which are often used in biology, mathematical chemistry, and psychology (Bonchev 1983, 2003; Diudea, Gutman, and Jantschi 2001; Sommerfeld 1994; Sommerfeld and Sobik 1994).

Approaches in Biology and Chemistry

In the beginning of the 1950s, there was considerable interest in applying information-theoretic concepts to scientific areas different from electrical engineering, language theory, and thermodynamics (Bonchev 2003; Shannon and Weaver 1997). Then, it turned out that the theoretical framework of information theory can also be very useful in investigating living systems, i.e., cell systems in the, at that time, emerging frontier area of applying information-theoretic concepts in biology. We notice that the first contributions in this area have been achieved by Morowitz (1953), Quastler (1953), Dancoff and Quastler (1953), Linshitz (1953), and

Rashewsky (1955). Thereby, Rashewsky (1955) made the first contribution regarding the determination of the structural information content of a graph. This contribution is based on finding distinguishable vertices and, then, to apply SHANNON's entropy formula to determine the information content. After this starting point, Mowshowitz (1968a–d) gave a pure mathematical treatment of this problem by using algebraic methods (Bonchev 2003). By using a certain equivalence criterion (utilizing vertex orbits), a graph-based system with n elements can be partitioned into k classes. Hence, a probability distribution can also be obtained that leads to the definition of an entropy of this system, i.e., its structural information content. Further, he defined a chromatic information content of a graph and examined graph operations like complement, sum, join etc., for investigating the change of the corresponding information measures.

Apart from biology, information-theoretic techniques have also been intensely applied in mathematical chemistry, e.g., to analyze and quantify the structural information content, the combinatorial complexity, and molecular branching of chemical graph structures (Bertz 1981, 1983; Bonchev 1979, 1983, 2003; Bonchev and Trinajstić 1977; Caporossi, Gutman, Hansen, and Pavlovi 2003; Diudea, Gutman, and Jäntschi 2001; Minoli 1975). The first rigorous and extensive treatment of so-called information indices used for quantifying structural information in chemical graphs has been stated by Bonchev (1979, 1983); Bonchev and Trinajstić (1977). To develop such indices, Bonchev (1983) has been using graph-theoretical quantities or other representations of structured objects to quantify structural information of graphs representing chemical structures. A short listing of known indices is now expressed as follows:

- Information indices based on topological characteristics, e.g., vertex orbits (Bonchev 1983; Mowshowitz 1968d; Rashewsky 1955; Trucco 1956).
- Information indices based on chromatic decompositions (Bonchev 1983; Harary 1969).
- Information indices based on adjacency matrices (Bonchev 1983).
- Information indices based on vertex degrees (Bonchev 1983).
- Information indices based on the incidence matrix of a graph (Bonchev 1983).
- Information indices based on cycle matrices of a graph (Bonchev 1983).
- Information indices based on distance matrices of graphs (Bonchev 1983).
- Information indices based on graph decompositions, e.g., the HOSOYA-graph decomposition (Bonchev 1983; Hosoya 1971).
- Centric indices and connectivity indices (Bonchev 1983).

As a direct consequence, Bonchev (2003) also used the above stated information indices for measuring the structural complexity of chemical molecule structures. For example, a possible definition for expressing the structural complexity states, the higher the information content of a (chemical) system, the more complex is the system (Bonchev 2003). Further definitions of so-called molecular complexity and results related to applying information-theoretical techniques to chemical graphs can be found in Bonchev (1983, 2003); Bonchev and Rouvray (2005). To finalize our short review on methods for measuring the structural information content of graphs in biology and chemistry, we now briefly outline a generalization of classical information indices recently introduced by Dehmer and Emmert-Streib (2008). In Dehmer and Emmert-Streib (2008), this entropy measure was mainly introduced for detecting molecular branching in chemical graphs. If we assume that $|V|$ denotes the number of vertices of a graph G, n denotes the number of different (obtained) sets of vertices, $|V_i|$ is the number of elements in the ith set of vertices, and we set $P_i = \frac{|V_i|}{|V|}$, then, SHANNON's entropy formulas can be stated as (Bonchev 1983):

$$I(G) = |V| \log(|V|) - \sum_{i=1}^{n} |V_i| \log(|V_i|) \tag{1}$$

or

$$I(G) = -\sum_{i=1}^{n} P_i \log(P_i). \tag{2}$$

We notice that Equation (2) now represents the mean information content of G. We clearly observe in Equations (1) and (2) that there are no free parameters or coefficients because, e.g., the quantities P_i are completely determined by the chosen partitioning (Dehmer and Emmert-Streib 2008). In contrast, we presented in Dehmer and Emmert-Streib (2008) the parametric entropy measure

$$I_{f^V}(G) := -\sum_{i=1}^{|V|} \frac{f^V(v_i)}{\sum_{j=1}^{|V|} f^V(v_j)} \log\left(\frac{f^V(v_i)}{\sum_{j=1}^{|V|} f^V(v_j)}\right), \tag{3}$$

where

$$f^V(v_i) := \alpha^{c_1|S_1(v_i,G)| + c_2|S_2(v_i,G)| + \cdots + c_{\rho(G)}|S_{\rho(G)}(v_i,G)|},$$
$$c_k > 0, \qquad 1 \le k \le \rho(G), \qquad \alpha > 0. \tag{4}$$

Here, $|S_j(v_i, G)|$ denotes the cardinality of a *j*-sphere of v_i regarding an undirected and connected graph G. $f^V(v_i)$ represents a so-called information functional that is based on metrical graph properties (Skorobogatov and Dobrynin 1988). Then, Equation (3) represents a family of parametric entropic measures. Following Dehmer and Emmert-Streib (2008), we have generalized the classical entropy measures for graphs represented by Equations (1) and (2) because we now have the possibility to weight certain structural characteristics of a graph. This can be done by varying the free parameters α and c_k. As an important remark, we want to notice that the local information spread in a graph can also be investigated by examining the ranges of α and c_k. In a subsequent section, we express the concept of an arbitrary information functional (Dehmer 2008a) and will give further examples for such functionals. As a result, we also obtain families of parametric graph entropy measures.

Approaches in Psychology

In the previous section, we gave a brief overview on methods to determine the structural information content of graphs which were mostly used in biology and mathematical chemistry. On the one hand, a main characteristic of the outlined methods is that the inferred or constructed graph structure can be considered as the result of a certain information process or communication between the elements of the underlying system. On the other hand, all shown methods dealt with the application of SHANNON's entropy formula (Shannon and Weaver 1997).

In this section, we briefly sketch a method for quantifying structural information of interpreted graphs, i.e., graphs with certain vertex and edge labels (Sommerfeld 1994; Sommerfeld and Sobik 1994). This method is not based on SHANNON's entropy formula and was originally designed for measuring structural information of so-called cognitive structures (Sommerfeld 1994; Sommerfeld and Sobik 1994). The first step to define such a method was to formalize a structure representing a piece of structural information (Sommerfeld 1994; Sommerfeld and Sobik 1994). This was done by using relational structures representing graphs. Second, a set of different interpretations was defined in the process of the formation of an internal representation based on a portion of external represented structural information (Sommerfeld and Sobik 1994). Hence, for measuring the structural information content of a cognitive structure represented by a graph, the introduction of an interpretation system was crucial. In Sommerfeld and Sobik (1994), an interpretation system describes relationships between external and internal information. As a result, the structural information content of a cognitive structure has been interpreted as the knowledge on the existence of certain relations

(based on edge and vertex labelings) between elements of this structure, i.e., the vertices of the graph. We want to emphasize that the application of this approach for measuring the structural information content does not result in a numerical value. In contrast, it is expressed by a set of interpretations (Sommerfeld and Sobik 1994). Further, it is important to mention that there exists a partial order between different pieces of structural information which are given by the relation of set inclusion (Sommerfeld and Sobik 1994). Starting from such a relation, in Sommerfeld and Sobik (1994), it was shown that it is now possible to compare certain portions of structural information. By applying this approach, it is not always possible to compare arbitrary portions of structural information because the defined structural information content depends on a chosen interpretation regarding the underlying structure (Sommerfeld and Sobik 1994). As a final remark, we now see that the just-mentioned definition (Sommerfeld and Sobik 1994) for expressing the structural information content of a graph is clearly distinct from the methods presented in the section on Approaches in Biology and Chemistry. These information measures were based on inferring a probability distribution to finally define the underlying topological entropy. Hence, for each unlabeled graph, the structural information content can be computed. In contrast, the definition of the structural information content we just outlined is not based on pure structural aspects only. The information content of a cognitive structure has been defined rather as a set of knowledge relations with respect to a chosen interpretation system (Sommerfeld and Sobik 1994).

ENTROPIC MEASURES FOR NETWORKS

We now present entropic measures based on graph decompositions to determine the structural information content of complex networks. For this, we first state some mathematical preliminaries (Buckley and Harary 1990; Cover and Thomas 2006; Godsil and Royle 2001; Harary 1969; Skorobogatov and Dobrynin 1988).

Mathematical Preliminaries

In this article we focus on undirected, connected graphs without loops and multiple edges. $G = (V, E), |V| < \infty, E \subseteq \binom{V}{2}$ denotes a finite, undirected and connected graph, e.g., see Figure 1. $\mathcal{G}_{UC}$ denotes the set of finite, undirected, and connected graphs. We call such a graph $G = (V, E)$ connected if for arbitrary vertices v_i and v_j there exists an undirected path
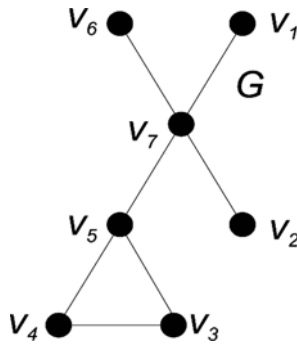
FIGURE 1 An undirected and connected graph *G*.

from v_i to v_j. 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. A graph $G \in \mathcal{G}_{UC}$ is called undirected tree if G is connected and cycle free. Further, an undirected rooted tree $T = (V, E)$ represents an undirected graph which possesses exactly one vertex $r \in V$ that is called root for which every edge is directed away from r. Hence, all vertices in T are uniquely accessible from r. The level of a vertex v in a rooted tree T is simply the length of the path from r to v. The path with the largest path length from the root to a leaf is denoted as h. In order to define graph entropy measures, we also need to introduce some metrical properties of graphs (Skorobogatov and Dobrynin 1988). $d(u,v)$ denotes the shortest distance between $u \in V$ and $v \in V$ where d is a metric.
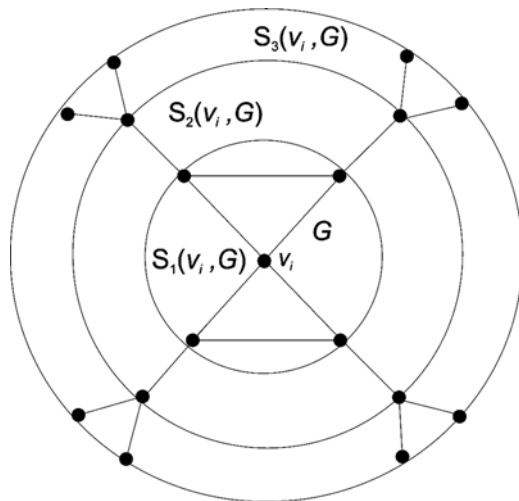

FIGURE 2 Visualized *j*-spheres of v_i, $j = 1, 2, 3$.

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. We call the set

$$S_j(v_i, G) := \{v \in V \mid d(v_i, v) = j, j \geq 1\}, \tag{5}$$

the j-sphere of v_i regarding G. $S_j(v_i, G)$ is simply the set of vertices whose distances to v_i equal j. As an example, Figure 2 shows the j-spheres $(j = 1, 2, 3)$ for a graph $G \in \mathcal{G}_{UC}$. Starting from the definition of j-spheres to obtain further information functionals, we define the local information graph of G that has been originally defined in Dehmer (2008a). This definition is based on the idea that certain information spreads out via shortest paths in a graph. Let $G = (V, E) \in \mathcal{G}_{UC}$. For a vertex $v_i \in V$, we define $S_j(v_i, G) = \{v_{u_j}, v_{w_j}, \ldots, v_{x_j}\}$ and the induced shortest paths,

$$P_1^j(v_i) = (v_i, v_{u_1}, v_{u_2}, \ldots, v_{u_j}),$$
$$P_2^j(v_i) = (v_i, v_{w_1}, v_{w_2}, \ldots, v_{w_j}),$$
$$\vdots \qquad\qquad\qquad \vdots$$
$$P_{k_2}^j(v_i) = (v_i, v_{x_1}, v_{x_2}, \ldots, v_{x_j}).$$

Their edge sets are defined by

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

By setting

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

and

$$E_{L_G} := E_1 \cup E_2 \cup \cdots \cup E_{k_j},$$

we define the local information graph $L_G(v_i, j)$ of G regarding v_i by
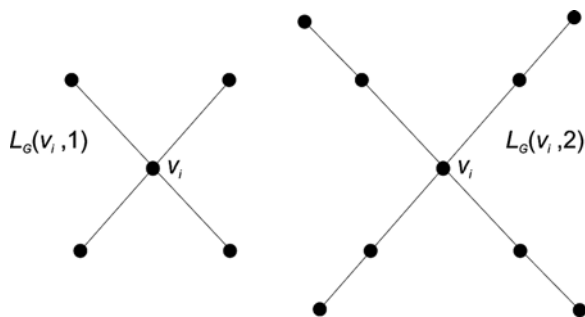
$$L_G(v_i, j) = (V_{L_G}, E_{L_G}). \tag{6}$$

FIGURE 3 Local information graphs of G (see Figure 2) regarding v_i, $j = 1, 2$.

Figure 3 shows the local information graphs $L_G(v_i, 1)$ and $L_G(v_i, 2)$. Its paths are induced by DIJKSTRA-distances (Dijkstra 1959). We want to emphasize that the local information graph regarding $v_i \in V$ cannot always be uniquely defined because often there exists more than one path from v_i to a certain vertex in the corresponding j-sphere (Dehmer 2008a). In order to introduce the classical entropy formally, we assume X to be a discrete random variable with alphabet A and $p(x_i) = \Pr(X = x_i)$ be the probability mass function of X. Finally, the entropy of X is defined by

$$H(X) := - \sum_{x_i \in A} p(x_i) \log(p(x_i))(x_i \in A). \tag{7}$$

Entropic Measures Based on Graph Decompositions

For example, in mathematics or computer science, the solution of many problems is based on the decomposition of objects for reducing the complexity of the given problem (Bosák 1990; Wheater and McCue 1992; Colbourn and Ling 2003). Starting from structured objects, one possibility to solve, e.g., a graph similarity problem, is to locally decompose the graphs under consideration into smaller graphs with a certain property, e.g., tress, etc. (Bosák 1990; Horváth, Gärtner, and Wrobel 2004; Emmert-Streib, Dehmer, and Kilian 2005). This aims to process the decomposed graphs more properly than the initial graphs. In this section, we present a method for determining the structural information content of graphs which is based on a graph decomposition. At this point, we want to point out that the problem of calculating the information content of a graph based on determining vertex partitions can be difficult and computationally inefficient, e.g., for large graphs. However, since our method is based on a tree decomposition of given graphs, we find that for tree-like graphs a vertex partitioning can be naturally obtained from the inferred level partitions. To introduce our method, we first express the definition of a
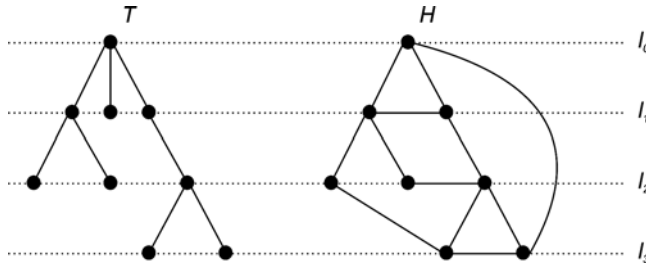
FIGURE 4 An ordinary rooted tree *T* and a generalized tree *H*. It holds $|L| = 4$ and $h = |L| - 1 = 3$.

(undirected) generalized tree representing a rooted tree-like structure (Dehmer and Emmert-Streib 2008). We remark that directed generalized trees have been introduced in Dehmer, Mehler, and Emmert-Streib (2008) and Mehler, Dehmer, and Gleim (2004).

Definition 3.1: Let $T = (V, E_1)$ be an undirected finite rooted tree. $|L|$ denotes the cardinality of the level set $L =: \{l_0, l_1, \ldots, l_h\}$. The longest length of a path in T is denoted as h. It holds $h = |L| - 1$. $\mathcal{L} : V \to L$ is a surjective mapping and it is called a multi-level function if it assigns to each vertex an element of the level set L. A graph $H = (V, E_{GT})$ is called a finite, undirected generalized tree if its edge set can be represented by the union $E_{GT} := E_1 \cup E_2 \cup E_3$, where

- E_1 forms the edge set of the underlying undirected rooted tree T.
- E_2 denotes the set of horizontal across-edges. A horizontal across-edge does not change a level i.
- E_3 denotes the set of edges which change at least one level.

Figure 4 shows a rooted tree T and a generalized tree H. We now describe the algorithm for uniquely decomposing a graph $G \in \mathcal{G}_{UC}$ into a set of undirected generalized trees (Emmert-Streib, Dehmer, and Kilian 2005).

Algorithm 3.1: A graph $G \in \mathcal{G}_{UC}$ with $|V|$ vertices can be locally decomposed into a set of generalized trees as follows: assign vertex labels to all vertices from 1 to $|V|$. These labels form the label set $L_S = \{1, \ldots, |V|\}$. Choose a desired height of the trees that is denoted by h. Choose an arbitrary label from L_S, e.g., i. The vertex with this label is the root vertex of a tree. Now, perform the following steps:

1. Calculate the shortest distance from vertex i to all other vertices in the graph G, e.g., by the algorithm of DIJKSTRA, see Cormen, Leiserson, and Rivest (1990) and Dijkstra (1959).
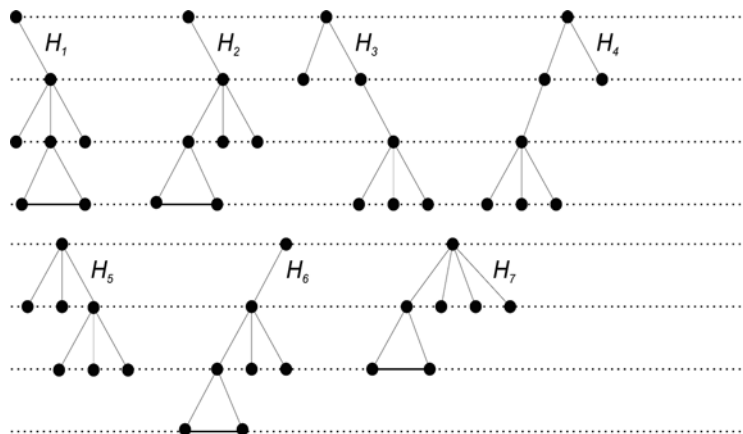
FIGURE 5 Result of the application of Algorithm (3.1) by using the graph of Figure 1. We set $h := \rho(G) = 3$.

2. The vertices with distance k are the vertices on the kth level of the resulting generalized trees. Select all vertices of the graph up to distance h, including the connections between the vertices. Connections to vertices with distance $> h$ are deleted.
3. Delete the label i from the label set L_S.
4. Repeat this procedure if L_S is not empty by choosing an arbitrary label from L_S; otherwise terminate.

Under the assumption that for all vertices of G, there exists a shortest path of length h, the application of Algorithm (3.1) results in a set S_G^H consisting of $|V|$ generalized trees with height h. Otherwise, the resulting tree set S_G^H contains generalized trees with $h_i < h$ where h_i denotes the resulting height of the ith generalized tree. Figure 5 shows the result of our decomposition method applied to the graph of Figure 1. Because one can easily observe that a vertex ordering on a certain level is generally not uniquely assignable, we therefore omitted in Figure 5 the vertex labels in the resulting generalized trees. We want to emphasize that to define the topological entropy of a generalized tree, such a vertex ordering on a generalized tree level is not necessarily required. In the following, we define the entropy of the decomposed generalized trees to measure the structural information content of a graph $G \in \mathcal{G}_{UC}$. A similar definition of a related graph class can be found in Emmert-Streib and Dehmer (2007b).

Definition 3.2: Let H be a generalized tree with height h. $|V|$ denotes the total number of vertices and $|V_i|$ denotes the number of vertices on the ith level, respectively. A probability distribution to H is assigned as follows: we set $p_i^V := |V_i|/(|V| - 1)$ Then, the vertex entropy of a generalized tree H is

defined by

$$I^V(H) := -\sum_{i=1}^{h} p_i^V \log(p_i^V). \tag{8}$$

From this definition, we see immediately that this entropy attains its maximum if H possesses the same number of vertices on each level $i, 1 \le i \le h$. As an example, H_5 depicted in Figure 5 has the maximal vertex entropy according to Definition 3.2. Correspondingly, we now define the edge entropy of a generalized tree H.

Definition 3.3: Let H be a generalized tree with height h. $|E|$ denotes the total number of edges and $|E_i|$ denotes the number of edges on the ith level, respectively. A probability distribution to H is assigned as follows: we set $p_i^E := \frac{|E_i|}{2|E|-\delta(r)}$. Then, the edge entropy of a generalized tree H is defined by

$$I^E(H) := -\sum_{i=1}^{h} p_i^E \log(p_i^E). \tag{9}$$

We observe that the edge entropy of a generalized tree H attains its maximum if H possesses the same number of edges on each level $i, 1 \le i \le h$. Figure 6 shows two generalized trees with maximal edge entropy according to Definition 3.3. Now, we are able to define the structural information content of a graph G by using the proposed decomposition method.

Definition 3.4: Let $G \in \mathcal{G}_{UH}$ and $S_G^H := \{H_1, H_2, \ldots, H_{|V|}\}$ be the associated set of generalized trees. We now define the structural information content of G by

$$I^V(G) := -\sum_{i=1}^{|V|} I^V(H_i). \tag{10}$$

and

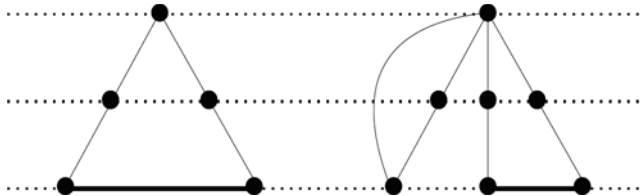$$I^E(G) := -\sum_{i=1}^{|V|} I^E(H_i). \tag{11}$$

FIGURE 6 Two generalized trees with maximal edge entropy.

Entropic Measures Based on Information Functionals

In this section, we generally present the concept of an arbitrary information functional (Dehmer 2008a) to quantify structural information in a network. Apart from the expressed information functional previously stated, we now give further examples for information functionals to demonstrate that this concept can be very useful for solving practical problems.

Information Functionals: Metrical Properties

Let $G \in \mathcal{G}_{UC}$ and let S be a certain set, e.g., a set of vertices or paths, etc. The mapping $f : S \to \mathbb{R}_+$ is called an information functional of G. It is always assumed that f is monotonous. To define a specific information functional that captures certain structural information of a given graph G, the set S has to be defined concretely. This leads to special information functionals, e.g., based on metrical properties, etc. We now start from an arbitrary graph $G \in \mathcal{G}_{UC}$ and define for $v_i \in V$ the quantities

$$p(v_i) := \frac{f(v_i)}{\sum_{j=1}^{|V|} f(v_j)}. \tag{12}$$

f represents an arbitrary information functional. We interpret the quantities $p(v_i)$ as vertex probabilities because

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

holds. Based on Equation (12), we therefore define the entropy of G as follows (Dehmer 2008a).

Definition 3.5: Let $G \in \mathcal{G}_{UC}$ and let f be an arbitrary information functional. We define the entropy of G by

$$I_f(G) := -\sum_{i=1}^{|V|} \frac{f(v_i)}{\sum_{j=1}^{|V|} f(v_j)} \log \left(\frac{f(v_i)}{\sum_{j=1}^{|V|} f(v_j)} \right). \tag{13}$$

In the following, we give some examples for information functionals. We already stated an information functional (see Equation (4)) which is based on vertex-sphere cardinalities, i.e., metrical properties of graphs. Another functional that is also based on metrical graph properties and uses the definition of the local information graph of G can be defined as follows (Dehmer 2008a).

Definition 3.6:   Let $G = (V, E) \in \mathcal{G}_{UC}$. For each vertex $v_i \in V$ and for $j = 1, 2, \ldots, \rho(G)$, we determine the local information graph $L_G(v_i, j)$, where $L_G(v_i, j)$ 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

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

expresses the sum of the path lengths associated to each $L_G(v_i, j)$. The information functional $f^P(v_i)$ is defined by

$$f^P(v_i) := \alpha^{b_1 l(P(L_G(v_i,1))) + b_2 l(P(L_G(v_i,2))) + \cdots + b_{\rho(G)} l(P(L_G(v_i, \rho(G))))}$$
$$b_k > 0, \qquad 1 \le k \le \rho(G), \qquad \alpha > 0. \tag{14}$$

b_k are arbitrary real positive coefficients.

In order to show that so-called local property measures (Dehmer 2008a) can also be used for defining information functionals, we express the following definition. Here, the information functional is based on an arbitrary vertex centrality measure (Brandes 2001; Sabidussi 1966; Wasserman and Faust 1994).

Definition 3.7: Let $G \in \mathcal{G}_{UC}$ and let $L_G(v_i, j)$ be the local information graph of G, for each vertex $v_i \in V$. We define $f^C(v_i)$ as

$$f^C(v_i) := \alpha^{a_1 \beta^L G^{(v_i,1)}(v_i) + a_2 \beta^L G^{(v_i,2)}(v_i) + \cdots + a_{\rho(G)} \beta_L G^{(v_i, \rho(G))}}(v_i),$$
$$\beta \le 1, \qquad a_k > 0, 1 \le k \le \rho(G), \qquad \alpha > 0. \tag{15}$$

β is an arbitrary vertex centrality measure and a_k are real positive coefficients.

We notice that the notation $\beta^{L_G(v_i,j)}(v_i)$ expresses we apply β to v_i regarding $L_G(v_i, j)$. Finally, by incorporating the defined information functionals, we obtain families of entropic graph measures, i.e.,

$$I_{f^V}(G) := -\sum_{i=1}^{|V|} \frac{f^V(v_i)}{\sum_{j=1}^{|V|} f^V(v_j)} \log\left(\frac{f^V(v_i)}{\sum_{j=1}^{|V|} f^V(v_j)}\right), \tag{16}$$

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

and

$$I_{f^C}(G) := -\sum_{i=1}^{|V|} \frac{f^C(v_i)}{\sum_{j=1}^{|V|} f^C(v_j)} \log\left(\frac{f^C(v_i)}{\sum_{j=1}^{|V|} f^C(v_j)}\right). \tag{18}$$

We remark that these entropy measures depend on the free parameter α and the coefficients of the just defined information functionals.

Information Functionals: Graph Decompositions
In a previous section, we introduced a method to measure the structural information content of a graph that is based on a graph decomposition. A generalized tree decomposition is a special kind of a graph decomposition which results in a set of generalized trees. For comparing the resulting entropies with those defined in the previous section, we now introduce further information functionals for generalized trees which also depend on a free parameter α. Hence, starting from a generalized tree decomposition of a graph $G \in \mathcal{G}_{UC}$, we also obtain two families of graph entropy measures. Finally, starting from example graphs, we compare the corresponding information contents numerically.

Definition 3.8: Let H be a generalized tree with height h. $|V_i|$ and $|E_i|$ denotes the number of vertices and edges on level $i, 0 \leq i \leq h$, respectively. For each level l_i, we define the information functionals

$$f_l^V(l_i) := \alpha^{|V_i|}, \qquad \alpha > 0, \tag{19}$$

and

$$f_l^E(l_i) := \alpha^{|E_i|}, \qquad \alpha > 0. \tag{20}$$

Definition 3.9: Let H be a generalized tree with height h. Then, the entropies $I_\alpha^V(H)$ and $I_\alpha^E(H)$ are defined by

$$I_\alpha^V(H) := -\sum_{i=0}^{h} \frac{f_l^V(l_i)}{\sum_{j=1}^{h} f_l^V(l_j)} \log\left(\frac{f_l^V(l_i)}{\sum_{j=1}^{h} f_l^V(l_j)}\right), \tag{21}$$

and

$$I_\alpha^E(H) := -\sum_{i=0}^{h} \frac{f_l^E(l_i)}{\sum_{j=1}^{h} f_l^E(l_j)} \log\left(\frac{f_l^E(l_i)}{\sum_{j=1}^{h} f_l^E(l_j)}\right), \tag{22}$$

respectively.

Starting from these definitions, Definition 3.4 can be now rewritten as follows.

Definition 3.10: Let $G \in \mathcal{G}_{UH}$ and $S_G^H := \{H_1, H_2, \ldots, H_{|V|}\}$ be the associated set of generalized trees. We obtain,

$$I^V(G) = \sum_{i=1}^{|V|} I_\alpha^V(H_i), \tag{23}$$

and

$$I^E(G) = \sum_{i=1}^{|V|} I_\alpha^E(H_i). \tag{24}$$

Complexity Analysis

In Dehmer (2008a), we have already analyzed the time complexities for calculating the entropies $I_{f^V}(G)$, $I_{f^P}(G)$, and $I_{f^C}(G)$. The result of this analysis can be summarized by expressing the following theorem (Dehmer 2008a).

Theorem 3.2: *For a graph $G \in \mathcal{G}_{UC}$, the time complexity to compute the entropies $I_{f^V}(G)$, $I_{f^P}(G)$, and $I_{f^C}(G)$ is $O(|V|^3)$.*

For the complexity analysis of the presented graph entropy approach which is based on the generalized tree decomposition, we see that we finally obtain a similar result. First, we get the following.

Proposition 3.3: *The time complexity for decomposing a graph $G \in \mathcal{G}_{UC}$ by using Algorithm 3.1 is $O(|V|^3)$.*

Proof: Starting from the definition of Algorithm 3.1, we have to compute all shortest paths in G. This can be done by determining all *j*-spheres, for all vertices $v_i \in V$. For computing all shortest distances, we can apply an existing shortest path algorithm, e.g., DIJKSTRA's algorithm (Dijkstra 1959) $|V|$ times for each vertex as a starting point. This procedure (Cormen, Leiserson, and Rivest 1990) requires time complexity $O(|V|^3)$.

Proposition 3.4: *The computation of the entropies $I_\alpha^V(H_i)$ and $I_\alpha^E(H_i)$ for all generalized trees H_i of S_G^H requires $O(\sum_{i=1}^{|V|} |V_{H_i}|^2)$.*

Proof: The creation and parsing process of the adjacency matrix of a generalized tree H_i requires $O(|V_{H_i}|^2)$ where V_{H_i} denotes the vertex set of H_i.

It holds $|S_G^H| = |V|$. This implies that performing this task $|V|$ times leads to

$$\sum_{i=1}^{|V|} O(|V_{H_i}|^2) = O\left(\sum_{i=1}^{|V|} |V_{H_i}|^2\right).$$

By combining the obtained results, we get a statement for the overall computational complexity to calculate the structural information content of $G \in \mathcal{G}_{UC}$, based on Algorithm 3.1.

Theorem 3.5: The overall time complexity to calculate $I^V(G)$ and $I^E(G)$ is finally $O(|V|^3 + \sum_{i=1}^{|V|} |V_{H_i}|^2)$.

Numerical Results

The aim of this section is to interpret the numerical results for comparing the resulting information contents by using certain example graphs. Starting from the graphs depicted in Figure 7, we calculated the structural information contents $I_{f^V}(G_i)$ and $I^V(G_i)$. To compute $I_{f^V}(G_i)$, we determined the corresponding j-spheres for all graphs and chose the c_k values such that $c_1 := 1, c_2 := 2, c_3 := 3, c_4 := 4$. In contrast, for calculating the entropies $I_{f^V}(G_i)$, we first decomposed all graphs that aimed to obtain their associated generalized tree sets $S_{G_1}^H, S_{G_2}^H$, and $S_{G_3}^H$. After determining the entropies $I_\alpha^V(H_i)$, we finally used Definition 3.10 to calculate the structural information contents for G_i. The plotted information contents $I_{f^V}(G_i)$ and $I^V(G_i)$ in dependence of the free parameter α are shown in Figure 8.

For interpreting these numerical results, we first consider the information contents $I_{f^V}(G_i)$. We start with the observation that $I_{f^V}(G_2)$ is almost everywhere larger than $I_{f^V}(G_1)$. Further, we see that $I_{f^V}(G_3)$ is constant and equals maximum entropy of a graph with five vertices. We notice that by incorporating the information functional f^V to determine Equation (16), it has been generally proven that the complete graph $K_{|V|}$ has always maximum entropy (Dehmer 2007b). We now interpret these results in such a way that we consider the graph G_3 as structurally more complex than G_2 and G_2 more complex than G_1. Starting from the definition of f^V, this interpretation can be explained by the fact that a stronger branching of
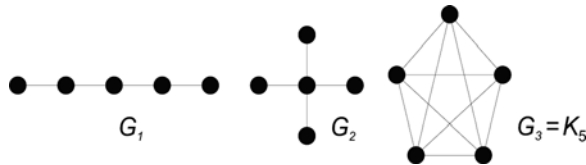

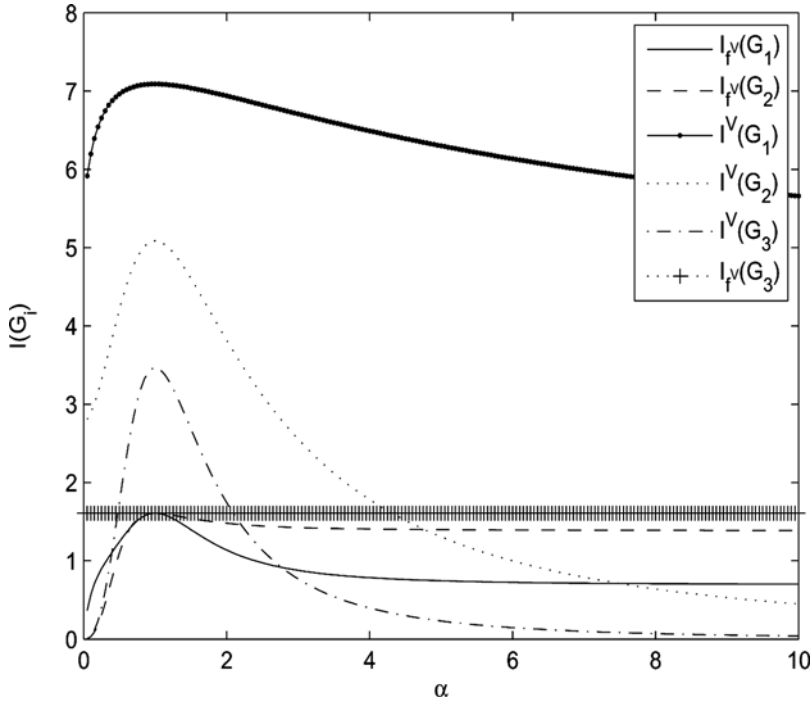**FIGURE 7** Example graphs $G_i \in \mathcal{G}_{UH}, i = 1, 2, 3$.

FIGURE 8 Structural information contents of G_1, G_2 and G_3.

a graph leads to larger values of the cardinalities of the corresponding *j*-spheres. Our results are in agreement with a statement of Bonchev (2003), that a complete graph should be considered as structurally complex than other graphs with the same number of vertices, e.g., chain or star graphs. In order to discuss the results by using Definitions 3.8 and 3.10, we see in Figure 8 that the resulting information contents now appear in reverse order, compared to those previously mentioned. By using the entropy definition that is based on a generalized tree decomposition, we now find that $I^V(G_1)$ is everywhere larger than $I^V(G_2)$ and $I^V(G_2)$ is everywhere larger than $I^V(G_3)$. This result can be understood by recalling Definitions 3.8 and 3.10 and examining the resulting decompositions $S_{G_1}^H$, $S_{G_2}^H$, and $S_{G_3}^H$. In particular, we found that two generalized trees of $S_{G_1}^H$ possess maximum entropy. Further, the vertex distribution of the resulting generalized tree set of G_2 is less homogeneous as in the case of G_1. The fact why $I^V(G_2)$ is everywhere larger than $I^V(G_3)$ can be similarly explained by examining the decompositions $S_{G_2}^H$ and $S_{G_3}^H$. Finally, we conclude from the obtained results that the structural information content of a graph can obviously not be consistently defined. The behavior of such an entropic measure clearly depends on the underlying definition and specific problem that needs to be examined.

SUMMARY

This article dealt with information-theoretic concepts for analyzing complex networks. In the first two sections, we gave a short overview about the topic. Then, we reviewed some known approaches to determine the structural information content of networks in biology, mathematical chemistry, and psychology. As an important remark, the so-called structural information content of a network was defined and interpreted as the resulting entropy of the underlying network topology. As a major contribution, we introduced a method for determining the structural information content of graphs that is based on a graph decomposition. Generally, the main idea of a decomposition method is to reduce the complexity of the given problem by decomposing the object under consideration into smaller parts which can be hopefully processed more properly. In detail, we decomposed an undirected and connected graph into so-called generalized trees to find naturally given vertex partitions. Starting from the resulting generalized tree sets, we expressed two methods to determine the structural information content of an undirected and connected graph. For comparing these entropy measures with those of the section entitled Entropic Measures Based on Information Functionals, we also defined a parametric version of the entropy measure that is based on the generalized tree decomposition. The numerical results by using some example graphs can be found in the section entitled Numerical Results. As an important result, we found that the computational complexity of the graph entropy approach based on the shown graph decomposition method is polynomial.

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