

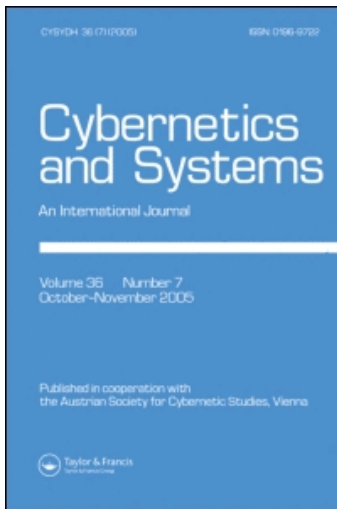
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Matthias Dehmer ^a; Stephan Borgert ^b

^a Center for Mathematics, University of Coimbra, Coimbra, Portugal ^b Darmstadt University of Technology, Telecooperation Group, Darmstadt, Germany

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CHARACTERIZING CLASSES OF STRUCTURED OBJECTS BY MEANS OF INFORMATION INEQUALITIES

MATTHIAS DEHMER¹ and STEPHAN BORGERT²

¹Center for Mathematics, University of Coimbra,
Coimbra, Portugal

²Darmstadt University of Technology, Telecooperation
Group, Darmstadt, Germany

The problem to characterize and investigate structured objects by using information theory is currently of considerable interest. In this article, we describe a method for characterizing structured objects representing graphs by means of information inequalities. For this, we deal with information inequalities that describe relations between information measures for graphs. Additionally, we sketch an approach for comparing such information measures qualitatively.

Keywords: Inequalities; Information content, Information measures, Structured objects

INTRODUCTION

In cybernetics, sociology, and computer science, the theory of structured objects provides powerful tools to represent structures and processes by means of graphs (Cook and Holder 2007; Hage and Harary 1995;

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Address correspondence to Matthias Dehmer, University of Coimbra, Center for Mathematics, Apartado 3008, 3001-45 Coimbra, Portugal. E-mail: dehmer@math.uc.pt

Jablonski and Lupanow 1980; Lewin 1936; Sobik 1982, 1986; Sommerfeld and Sobik 1994; Sommerfeld 1994; Wasserman and Faust 1994). By structured objects, we refer to objects that can be represented by relational algebras. If one restricts to the analysis of two-digit relations, such relational objects can be easily described by graphs (Harary 1969; Sobik 1986).

In this article, we want to address the abstract question to characterize classes of structured objects by using information inequalities. In our case, an information inequality describes a relation between information measures for graphs. In terms of dealing with structured objects, information theory (Aczél and Daróczy 1975; Shannon and Weaver 1997) offers a lot of quantitative methods to investigate information processing and information transmission in graphs (Dehmer 2007; Solé and Valverde 2004). In particular, if we want to characterize structured objects as well as classes of those by applying information measures, we have to answer the question to which aspect of information we are referring to, e.g., structural information or semantic information. Throughout this article, if we speak about abstract information measures for graphs, we always use the concept of structural information (Dehmer 2007; Mowshowitz 1968a–d; Rashewsky 1955; Solé and Valverde 2004), e.g., by inferring structural characteristics of graphs (Doro-govtsev and Mendes 2003; Skorobogatov and Dobrynin 1988). Then, this task is equivalent to measure the so-called structural information content (Bonchev 1983; Mowshowitz 1968d) of a graph representing the entropy of the underlying graph topology (Bonchev 2003; Dehmer 2007; Mowshowitz 1968d). This article aims to outline an approach for characterizing classes of structured objects by means of information inequalities. We will finally say that a class of structured objects is characterized by a certain information measure if for each pair of graphs a certain (information) inequality holds. One possibility to do so is to apply a given information measure for quantifying the information content of such a graph. As a result, we get a system of information inequalities. Another possibility is to infer such inequalities theoretically.

MATHEMATICAL PRELIMINARIES

In the following, we first express some graph-theoretical and information-theoretic definitions (Aczél and Daróczy 1975; Harary 1969; Dehmer, Emmert-Streib, and Gesell 2008; Harary 1969; Shannon and Weaver 1997; Sobik 1986).

Definition 2.1. Let A_1, A_2, \dots, A_n be arbitrary sets. Then, an n -digit relation R is a subset of the Cartesian product of the corresponding sets A_1, A_2, \dots, A_n , i.e.,

$$R \subseteq A_1 \times A_2 \times \dots \times A_n, \tag{1}$$

and

$$A_1 \times A_2 \times \dots \times A_n := \{(a_1, a_2, \dots, a_n) | a \in A_1, a_2 \in A_2, \dots, a_n \in A_n\}. \tag{2}$$

Definition 2.2. Let V be the set of elementary objects. Let E be an n -digit relation (n) between the elementary objects of V . We call $O := (V, E)$ a general, finite structured object if $|V| < \infty, V \neq \emptyset$ and $E \subseteq V \times V \times \dots \times V$.

Definition 2.3. Let V be the set of elementary objects which we call vertices. Let E be a 2-digit relation between the vertices of V . If O is defined as $O := (V, E), |V| < \infty, V \neq \emptyset$ and $E \subseteq V \times V$, we call O a finite directed graph. In contrast, if it holds $O := (V, E), |V| < \infty, E \subseteq \binom{V}{2}$, we call O a finite undirected graph.

Definition 2.4. Let $(\Delta_n)^k, \mathbb{N} \ni n \geq 2$ be the set

$$(\Delta_n)^k := \left\{ P = (p_1, p_2, \dots, p_n) \mid p_i \in [0, 1]^k, i = 1, 2, \dots, n, \sum_{i=1}^n p_i = 1 \right\}. \tag{3}$$

The addition of the vectors is defined componentwise and $\underline{1}$ denotes the k -dimensional vector $(1, 1, \dots, 1)^T$. The sequence of functions

$$I_n : (\Delta_n)^k \longrightarrow \mathbb{R} \tag{4}$$

is called a k -dimensional information measure. If $k = 1$,

$$I_n : (\Delta_n)^1 \longrightarrow \mathbb{R} \tag{5}$$

are called entropies.

CHARACTERIZATION OF STRUCTURED OBJECTS: INFORMATION INEQUALITIES

In this section, we propose an approach to characterize classes of structured objects by using information inequalities. For this, we assume C to

be a certain class of directed or undirected graphs. Further, we now set $k = 1$ and define the domain of Eq. (5) as C because we interpret the quantities p_1, p_2, \dots, p_n as probability values inferred from the structured objects under consideration. That means for a given $G \in C$, we first derive probability values p_1, p_2, \dots, p_n associated to G . Finally, this implies that $I_n(G) \in \mathbb{R}$ quantifies structural information of G . In the following, we always write $I(G)$ instead of $I_n(G)$ because we apply such information measures to structured objects of different orders. Starting from these preliminaries, we now state the main definition.

Definition 3.1. Let C be a class of directed or undirected graphs. We say that C is characterized by an information measure $I : C \rightarrow \mathbb{R}$ iff for each possible pair (G, H) with $G \neq H$ the inequality system

$$I(G) \underset{(<)}{\geq} I(H), \tag{6}$$

holds.

Example 3.1. We consider the graph class C depicted in Figure (1). Now, to quantify structural information of these graphs, we exemplarily apply the following information measure (Emmert-Streib and Dehmer 2007): Because a rooted tree T can be naturally divided into horizontal levels representing vertex partitions, we define the probability value for each level i by

$$p_i^V := \frac{|V_i|}{|V| - 1}, \tag{7}$$

$1 \leq i \leq h$. Starting from $T \in C$, $|V|$, denotes the total number of vertices, $|V_i|$ denotes the number of vertices on the i th level, and h denotes the height of T , respectively. Then, the vertex entropy of a rooted tree T is defined by using the SHANNON-entropy (Shannon and Weaver 1997)

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

We yield

$$I^V(T_1) = \log(3) = 1.5850 \text{ bits}, \tag{9}$$

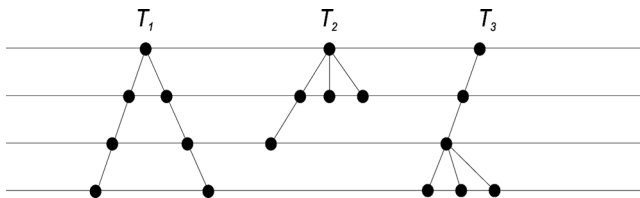


Figure 1. A graph class $C := \{T_1, T_2, T_3\}$. Each H_i represents a rooted tree.

$$I^V(T_2) = -\frac{3}{4} \log\left(\frac{3}{4}\right) - \frac{1}{4} \log\left(\frac{1}{4}\right) = 0.8113 \text{ bits}, \tag{10}$$

$$I^V(T_3) = -\frac{2}{5} \log\left(\frac{1}{5}\right) - \frac{3}{5} \log\left(\frac{3}{5}\right) = 1.3710 \text{ bits}, \tag{11}$$

where we took the logarithm to the base 2. Finally, we get the inequality system

$$I^V(T_1) > I^V(T_2), \tag{12}$$

$$I^V(T_1) > I^V(T_3), \tag{13}$$

$$I^V(T_2) < I^V(T_3). \tag{14}$$

Example for Inferring Information Inequalities

In the previous section, we claimed that C is characterized by an information measure I iff a certain inequality system holds. In Example (3.1), we applied a special information measure to characterize the given class C . As a direct consequence, we got the inequality system described by the inequalities (12)–(14). In contrast, we now show that it is also possible to infer information inequalities for graphs theoretically. For giving an example, we state the following assertions that have been recently proven in Dehmer (2008).

Theorem 3.2. *Let C be a class of directed or undirected graphs. Further, let $G = (V_G, E_G) \in C$ and $H = (V_H, E_H) \in C$ be non-isomorphic graphs. If $|G| > |H|$ and the following system of vertex probabilities*

$$\begin{aligned} p(\bar{v}_{j_1}, G) &> p(v_{i_1}, H), \\ p(\bar{v}_{j_2}, G) &> p(v_{i_2}, H), \\ &\vdots \\ p(\bar{v}_{j_{|V_H|}}, G) &> p(v_{i_{|V_H|}}, H), \\ p(\bar{v}_{j_{|V_H|+1}}, G) &> p(v_{\mu_1}, H), \\ &\vdots \\ p(\bar{v}_{j_{|V_G|}}, G) &> p(v_{\mu_k}, H), \end{aligned} \tag{15}$$

holds, then we obtain the information inequality

$$I(G) < I(H) + d_1, \quad d_1 > 0, \tag{16}$$

where

$$d_1 := - \sum_i^k p(v_{\mu_i}, H) \log(p(v_{\mu_i}, H)). \quad (17)$$

If $|G| < |H|$, the relation symbol in Inequality System (15) must be changed to “ $<$ ”. Then, we infer

$$I(G) + d_2 > I(H), \quad d_2 > 0, \quad (18)$$

where

$$d_2 := - \sum_i^k p(\bar{v}_{\mu_i}, G) \log(p(\bar{v}_{\mu_i}, G)). \quad (19)$$

Starting from Theorem (3.2), we also get the following assertion.

Theorem 3.3. *It holds*

$$I(G) > I(H) \quad \text{or} \quad I(G) < I(H) \quad \text{or} \quad I(G) = I(H). \quad (20)$$

We notice that in Theorems (3.2) and (3.3), the information measures $I(G)$ and $I(H)$ represent the corresponding SHANNON-entropies for graphs. We interpret these statements in a way that one is able to predict information inequalities for structured objects by assuming certain constraints. As constraint, we here chose an inequality system that describes relations between the vertex probabilities (Dehmer 2008).

QUALITATIVE ANALYSIS OF INFORMATION MEASURES

This section aims to give an example to define a method for performing a qualitative analysis of information measures to characterize graphs. A similar approach has been defined in Sobik (1986) for the qualitative comparison of graph similarity measures. In general, while doing a quantitative analysis means to examine numerical differences between information measures, a qualitative analysis examines relationships between the used information measures starting from a class of structured objects. First, that means we identify the pairs of structured objects (G, H) for which, e.g., $I(G) \geq I(H)$ holds. This procedure results in a graph where the set of vertices equals C , whereas two vertices will be connected by an edge iff for the corresponding information measures

the relation “ \geq ” holds. Second, if we apply this procedure to the same class C by using a different information measure \bar{I} , one can finally compare I and \bar{I} qualitatively by comparing the resulting graphs structurally (Bunke and Neuhaus 2007; Sobik 1986).

Definition 4.1. Let C be a class of directed or undirected graphs and let $I : C \rightarrow \mathbb{R}$ be an information measure. We define the directed graph

$$G^I = (V^I, E^I), \tag{21}$$

by setting $V^I = C$ and

$$E^I := \{(G, H) \mid G \neq H, I(G) \geq I(H)\}. \tag{22}$$

Example 4.1. Once again, we look at the trees shown in Figure 1. Similarly to Information Measure (8), we define the edge entropy of a tree as follows (Emmert-Streib and Dehmer 2007). Let T be a rooted tree with height h . $|E|$ denotes the total number of edges and $|E_i|$ denotes the number of edges on the i th level, respectively. Now, we set

$$p_i^E := \frac{|E_i|}{2|E| - \delta(r)}. \tag{23}$$

Then, the edge entropy of T is defined by

$$I^E(H) := - \sum_{i=1}^h p_i^E \log(p_i^E). \tag{24}$$

By using this information measure, we obtain

$$I^E(T_1) = -\frac{4}{5} \log\left(\frac{2}{5}\right) - \frac{1}{5} \log\left(\frac{1}{5}\right) = 1.5219 \text{ bits}, \tag{25}$$

$$I^E(T_2) = -\frac{4}{5} \log\left(\frac{4}{5}\right) - \frac{1}{5} \log\left(\frac{1}{5}\right) = 0.7219 \text{ bits}, \tag{26}$$

$$I^E(T_3) = -\frac{2}{9} \log\left(\frac{2}{9}\right) - \frac{4}{9} \log\left(\frac{4}{9}\right) - \frac{3}{9} \log\left(\frac{3}{9}\right) = 1.5305 \text{ bits}. \tag{27}$$

Finally, we obtain the same inequality system, i.e.,

$$I^E(T_1) > I^E(T_2), \tag{28}$$

$$I^E(T_1) > I^E(T_3), \tag{29}$$

$$I^E(T_2) < I^E(T_3), \tag{30}$$

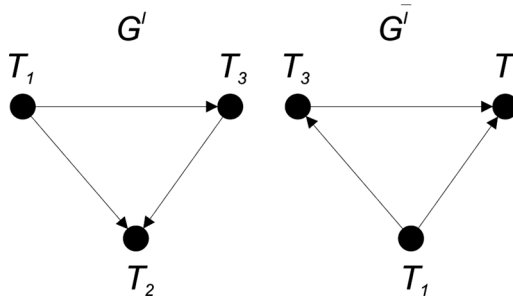


Figure 2. The resulting graphs G^I and $G^{\bar{I}}$ for comparing I and \bar{I} qualitatively.

If we now apply Definition (4.1) to T_1 , T_2 , and T_3 , we get the graphs G^I and $G^{\bar{I}}$ which are depicted in Figure (2) for comparing I^V and I^E qualitatively. In this case, we see that the obtained graphs are isomorphic.

SUMMARY AND CONCLUSION

This article dealt with suggesting a method to characterize classes of structured objects by means of information inequalities. By using an information measure that quantifies structural information of a graph, we called a graph class characterized by an information measure iff for each possible pair of graphs a certain information inequality holds. In the present article, we outlined two possibilities to do so. First, we started with a special information measure and calculated the corresponding inequality system. The second possibility we sketched to characterize structured objects by means of information inequalities was to infer such relations theoretically. For this, we expressed an example for a method to generate information inequalities starting from certain constraints.

In the future, we want to investigate different kinds of information measures to characterize large sets of graphs.

REFERENCES

- Aczel, J. and Daróczy, Z. 1975. *On measures of information and their characterizations*. Academic Press, New York, London.
- Bonchev, D. 1983. *Information theoretic indices for characterization of chemical structures*. Chichester: Research Studies Press.

- Bonchev, D. 2003. *Complexity in chemistry. Introduction and fundamentals*. Philadelphia: Taylor and Francis.
- Bunke, H. and Neuhaus, M. 2007. Graph matching: Exact and error-tolerant methods and the automatic learning of edit costs. In *Mining graph data*, edited by D. Cook and L. B. Holder. Wiley-Interscience, Hoboken, New Jersey, pp. 17–32.
- Cook, D. and Holder, L. B. 2007. *Mining graph data*. Wiley-Interscience.
- Dehmer, M. 2007. Information processing in complex networks: Graph entropy and information functionals. *Applied Mathematics and Computation* 201 (1–2): 15, 2008 pages 82–94.
- Dehmer, M. 2008. Relations between the topological complexities of complex networks. In *Proceedings of the 2008 International Conference on Machine Learning: Models, Technologies & Applications (MLMTA'08)*. Las Vegas, NV, pages 885–858.
- Dehmer, M., Emmert-Streib, F., and Gesell, T. 2008. A comparative analysis of multidimensional features of objects resembling sets of graphs. *Applied Mathematics and Computation* 196: 221–235.
- Dorogovtsev, S. N. and Mendes, J. F. F. 2003. *Evolution of networks. From biological networks to the Internet and WWW*. Oxford University Press.
- Emmert-Streib, F. and Dehmer, M. 2007. Information theoretic measures of UHG graphs with low computational complexity. *Applied Mathematics and Computation* in press.
- Hage, P. and Harary, F. 1995. Eccentricity and centrality in networks. *Social Networks* 17: 57–63.
- Harary, F. 1969. *Graph theory*. Addison Wesley Publishing Company.
- Jablonski, S. W. and Lupanow, O. B. 1980. Diskrete Mathematik und mathematische Fragen der Kybernetik. *Lehrbücher und Monographien aus dem Gebiete der exakten Wissenschaften: Mathematische Reihe*, Volume 71. Birkhauser Publishing.
- Lewin, K. 1936. *Principles of topological psychology*. New York: McGraw-Hill.
- Mowshowitz, A. 1968a. Entropy and the complexity of graphs ii: The information content of digraphs and infinite graphs. *Bull. Math. Biophys.* 30: 225–240.
- Mowshowitz, A. 1968b. Entropy and the complexity of graphs iii: Graphs with prescribed information content. *Bull. Math. Biophys.* 30: 387–414.
- Mowshowitz, A. 1968c. Entropy and the complexity of graphs iv: Entropy measures and graphical structure. *Bull. Math. Biophys.* 30: 533–546.
- Mowshowitz, A. 1968d. Entropy and the complexity of the graphs i: An index of the relative complexity of a graph. *Bull. Math. Biophys.* 30: 175–204.
- Rashewsky, N. 1955. Life, information theory, and topology. *Bull. Math. Biophys.* 17: 229–235.
- Shannon, C. E. and Weaver, W. 1997. *The mathematical theory of communication*. University of Illinois Press.

- Skorobogatov, V. A. and Dobrynin, A. A. 1988. Metrical analysis of graphs. *MATCH* 23: 105–155.
- Sobik, F. 1982. Graphmetriken und Klassifikation strukturierter Objekte. *ZKI-Informationen, Akad. Wiss. DDR* 2(82): 63–122.
- Sobik, F. 1986. Modellierung von Vergleichsprozessen auf der Grundlage von Ähnlichkeitsmaßen für Graphen. *ZKI-Informationen, Akad. Wiss. DDR* 4: 104–144.
- Solé, R. V. and Valverde, S. 2004. Information theory of complex networks: On evolution and architectural constraints. *Lecture Notes in Physics* 650: 189–207.
- Sommerfeld, E. 1994. *Kognitive Strukturen. Mathematisch-psychologische Elementaranalysen der Wissensstrukturierung und Informationsverarbeitung*. Waxmann Publishing.
- Sommerfeld, E. and Sobik, F. 1994. Operations on cognitive structures – their modeling on the basis of graph theory. In *Knowledge structures*, edited by D. Albert. Springer, pp. 146–190.
- Wasserman, S. and Faust, K. 1994. *Social network analysis: Methods and applications*. Structural Analysis in the Social Sciences. Cambridge University Press.