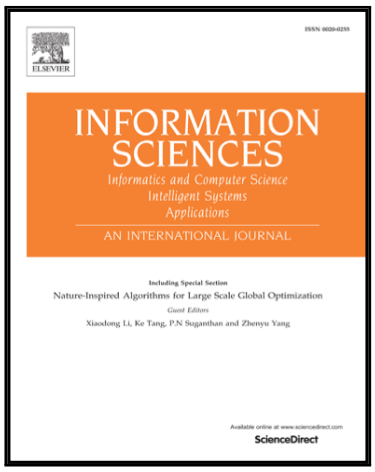

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PII: S0020-0255(18)30598-X
DOI: https://doi.org/10.1016/j.ins.2018.07.072
Reference: INS 13839

To appear in: *Information Sciences*

Received date: 10 May 2017
Revised date: 12 July 2018
Accepted date: 29 July 2018

Please cite this article as: Matthias Dehmer, Zengqiang Chen, Frank Emmert-Streib, Yongtang Shi, Shailesh Tripathi, Graph Measures With High Discrimination Power Revisited: A Random Polynomial Approach, *Information Sciences* (2018), doi: https://doi.org/10.1016/j.ins.2018.07.072

Graph Measures With High Discrimination Power Revisited: A Random Polynomial Approach

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Abstract

Finding graph measures with high discrimination power has been triggered by searching for so-called complete graph invariants. In a series of papers, we have already investigated highly discriminating measures to distinguish graphs (networks) based on their topology. In this paper, we propose an approach where the graph measures are based on the roots of random graph polynomials. The polynomial coefficients have been defined by utilizing information functionals which capture structural information of the underlying networks. Our numerical results obtained by employing exhaustively generated graphs reveal that the new approach outperforms earlier results in the literature.

Keywords: Quantitative Graph Theory, Networks, Statistics, Graphs, Data Science
2000 MSC: 62D99, 05C75, 68R10, 90B10

1. Introduction

The search for complete graph invariants has been an exciting and stimulating problem in mathematics and computer science, see [3, 8, 48, 47]. A graph invariant is a quantitative measure [2, 49] capturing structural information of an underlying network which is invariant under isomorphism. Hence, the problem of finding complete graph invariants is instantaneously connected to the graph isomorphism problem whose complexity is still not known for general graphs, see [36, 46]. So far, no complete graph invariant for the general case has been found. Yet, complete graph invariants for special cases and graph classes have been identified and their properties have been explored. For example, see [8]. Suppose, a given graph invariant is complete for a set of pairwisely non-isomorphic graphs. That means, the invariant structurally discriminates all graphs uniquely. Thus, finding highly discriminating graph measures may also lead to complete or almost complete graph invariants.

We briefly survey some related work when it comes to investigate the discrimination power of graph measures. In fact, the degeneracy is an undesirable property of a graph measure, see [49] as in theory, non-isomorphic graphs should have different measured values. To the best of our knowledge, the first study of the discrimination power of a graph measure relates to discriminate structural differences between isomers in the context of computational chemistry [4]. After this, Balaban [1] developed the Balaban J index which has high discrimination power (i.e., low degeneracy) for chemical trees. Dehmer et al. [11] demonstrated that the Balaban J index is highly

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