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Highly unique network descriptors based on the roots of the permanental polynomial

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ABSTRACT

In this paper, we examine the zeros of permanental polynomials as highly unique network descriptors. We employ exhaustively generated networks and demonstrate that our defined graph measures based on the moduli of the zeros of permanental polynomials are quite efficient when distinguishing graphs structurally. In this work, we continue with a line of research that relates to the search of almost complete graph invariants. These highly unique network measures may serve as a powerful tool for tackling graph isomorphism.

1. Introduction

Methods for analyzing complex networks have been ubiquitous since many years [9,10,37,38]. The main reason comes from the fact that various mathematical and related problems can be translated into a network-based description. Choosing the right method for a particular problem has been intricate, see [10]. Therefore we already elaborated on the problem that graphs can be analyzed descriptively or quantitatively, see [10]. The descriptive analysis of networks mostly corresponds to problems in classical graph theory, see Halin [20] or Harary [21]. In this paper, we focus on a special aspect when dealing with the latter problem. We put the emphasis on discriminating networks uniquely when using quantitative network

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measures. This general problem has already been tackled by Dehmer and co-workers [12,14,15] and many other contributors, see, e.g., [1,3,26,42].

In order to define structural graph measures to characterize networks quantitatively, it has not been clear which graph invariant turns out to be optimal. Yet, this choice depends on the underlying network problem. For instance, eigenvalue-based measures turned out to be highly efficient when discriminating networks uniquely, see [14]. This task is based on computing single network measures where a single network measure characterizes a given network quantitatively. These measures are often called topological indices, see [25,28]. Another task relates to compare networks structurally by using similarity or distance measures [11,17]. Being aware of the just mentioned problem, Dehmer et al. [13] performed a large scale study to examine which graph invariant and what kind of graph measures have the highest uniqueness when applying them to exhaustively generated graphs. In the already mentioned papers, see [14], we have explored the problem to define unique eigenvalue-based measures extensively. For example, we used the moduli of the roots of several known graph polynomials to define certain graph measures which turned out to be meaningful and efficient. Also, we employed the Randić matrix [14] to define graph polynomials whose moduli of their zeros were good candidates to define highly discriminating graph measures. An overview and facts on graph eigenvalues and eigenvalue-based graph measures and their properties can be found in, e.g., [8,14,18,28,40,43].

The paper is in the line of the foregoing ones, see [14,15]. In particular, we demonstrate that a rather simple polynomial-based representation achieves very good results when discriminating exhaustively generated graphs structurally. We will see that the graph measures which are based on the moduli of the zeros of the permanental polynomial turned out to be quite efficient and, in parts, they outperform the foregoing measures defined in [14,15]. A further reason why we have chosen the permanental polynomial of a graph is that it has yet been relatively unexplored, see [24]. Theoretical insights and practical experience about the zeros of the permanental polynomial of a graph will be surely helpful in Quantitative Graph Theory [10]. We provide a brief review on the permanental polynomial in the next section.

2. Methods and results

2.1. The permanental polynomial of a graph

Similar to the characteristic polynomial of a graph [8], the *permanental polynomial* of a graph $G = (V, E)$ has been defined by [29,30,36]

$$P_{\text{per}}^{M(G)}(z) := \text{per}(zE - M(G)) = \sum_{i=0}^{|V|} a_i z^i. \tag{1}$$

$M(G) = (m_{ij})_{ij}$ is a $|V| \times |V|$ square matrix which encodes structural information of the graph G. For example, $M(G) = A(G)$ or $M(G) = D(G)$ means that we consider the adjacency matrix A [21] or the distance matrix D [16,21] of a given graph G.

The permanent of the matrix $M(G)$ has been defined by [29,30,36]

$$\text{per}(M(G)) = \sum_{\sigma} \prod_{i=1}^{|V|} m_{i\sigma(i)}, \tag{2}$$

where the summation goes over all the permutations σ of $\{1, 2, \ldots, |V|\}$. According to Li et al. [27], we observe that the permanent of the matrix has been defined similarly compared to the determinant. However, the different definition of the permanent clearly results in a different polynomial representation compared by only using the determinant [8]. Computational challenges when determining the permanent numerically have also been discussed by Li et al. [27]. Following [27], no algorithm has yet been found to calculate the determinant of a matrix efficiently. To see how we tackle this problem practically, see Section 2.3.1.

Particularly, the permanental polynomial of graphs have been investigated in mathematical chemistry. In a series of papers, Cash [4–7] explored interrelations between the permanent of the adjacency matrix and the structure of chemical graphs. Earlier work is due to Gutman [19] when examining relationships between the permanent of the adjacency matrix of a chemical graph and their Kekulé structures. To study the existing body of literature related to permanent polynomials, we refer to the up-to-date review due to Li et al. [27].

In terms of investigating the zeros of the permanental polynomial, we also refer to Cash [4]. More precisely, he explored clusters of the zeros of the permanental polynomial of a isomer series of fullerenes [4]. In particular, Cash [4] examined the variation of the zeros in terms of the size of the fullerenes. More recent work in this context is due to Tong et al. [44] when considering the same problem for larger fullerenes. This proves that the zeros of the permanental polynomial encode structural information meaningfully by considering special graph classes.

The question we are going to tackle in this paper relates to the problem whether the zeros of permanental polynomials are suitable to discriminate graphs uniquely. We emphasize that this problem does not only depend on the zeros of a particular graph polynomial. The considered graph class also matters and the way how we use the zeros to define a graph measures. With other words, the uniqueness of the resulting graph measures also depends on the type of graph measure. Note that we have already investigated this problem by employing well-known graph measures like the Balaban J index and graph entropies, see [13]. In this paper and in [14,15], we use the basic form of the graph measures as defined in