The Uniqueness of $D_{MAX}$-Matrix Graph Invariants

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Abstract

In this paper, we examine the uniqueness (discrimination power) of a newly proposed graph invariant based on the matrix $D_{MAX}$ defined by Randić et al. In order to do so, we use exhaustively generated graphs instead of special graph classes such as trees only. Using these graph classes allow us to generalize the findings towards complex networks as they usually do not possess any structural constraints. We obtain that the uniqueness of this newly proposed graph invariant is approximately as low as the uniqueness of the Balaban $J$ index on exhaustively generated (general) graphs.

Introduction

Matrix-based descriptors have been developed extensively [1–3]. As a result, the distance matrix, the adjacency matrix and other graph-theoretical matrices [4] have been used to define topological graph measures and to examine their properties [4,5]. A property which has been of considerable interest when designing topological descriptors is referred to as uniqueness [6–8]. Generally, the uniqueness of a structural graph measure relates to the ability to distinguish the structure of non-isomorphic graphs uniquely. From a mathematical point of view, the low uniqueness or high degeneracy of a graph measure under consideration is an undesired aspect as non-isomorphic graphs should be mapped to non-equal values. Such a highly discriminating graph invariant could be then used to distinguish graph structures uniquely and, thus, to perform graph isomorphism testing [9,10]. In the context of graph isomorphism testing, so-called complete graph invariants have been investigated [9,11]. Such a graph invariant has the property that it discriminates all non-isomorphic graphs uniquely (i.e., without any degeneracy) and isomorphic graphs are mapped to equal values [9,11]. For example, Liu and Klein [11] made an attempt to derive complete graph invariants by using eigenvalues. Dehmer et al. [8,9] defined graph entropies which turned out to be the most discriminative measures so far when using exhaustively generated graphs. Clearly, such measures are suitable candidates to test graph isomorphism efficiency [9].

Recently, Randić et al. [2,12] defined so-called $D_{MAX}$ matrices and also topological descriptors thereof. Let $G = (V,E)$ be a finite graph. Then these matrices have been defined by using the ordinary distance matrix $D$ of $G$ such that in each row and column the dominant (largest) distances are used where other elements $eD$ are set to be zero, see [2,12]. Moreover they defined a new topological index $j$ which has the same definition than the well-known Balaban index $J$ [13] but uses $D_{MAX}$ instead of only using $D.$ Then based on example calculations, Randić et al. [2] argued that $j$ may be a promising candidate for isomorphism testing, but they did not examine the problem in depth on wider classes of graphs.

In this paper, we explore the uniqueness of $j$ by employing $D_{MAX}$ on a large scale. For this, we use exhaustively generated graphs with 9 and 10 vertices each [8] and alkane trees $T = (V_T,E_T)$ where $19 \leq |V_T| \leq 22.$ Our findings (see section 'Methods and Results') reveal that the uniqueness of $j$ is always worse than the one of $J$ and, thus, the uniqueness of $j$ is insufficient for performing isomorphism testing.

Methods and Results

The Structural Descriptors $J$ and $j$

Let $G = (V,E)$ be a finite graph. To define the Balaban index $J$ [13,14] of $G,$ let $(D)_{ij} := (d(v_i,v_j))_{ij}$ be the distance matrix. $d(v_i,v_j)$ is the topological distance between $v_i \in V$ and $v_j \in V.$ For each vertex $v_i \in V,$ $D_{Si}$ denotes the distance sum (row or column sum) by adding the entries in the corresponding row or column of $D.$ Let $\mu := |E|+1−|V|$ be the cyclomatic number [14]. Then $J$ has been defined by [13]

$$J(G) := \frac{|E|}{\mu + 1} \sum_{(v_i,v_j) \in E} |D_{Si}D_{Sj}|^{-\frac{1}{2}}.$$  \hspace{1cm} (1)

A critical analysis to examine the uniqueness of $J$ and other quantities has recently been carried out by Dehmer et al. [8] based on using exhaustively generated (general) graphs. In this sense Dehmer et al. examined the limitations of the Balaban $J$ index and found that this index is quite unstable [9]; here that means there is a strong dependency between the sample size of the graph set and the uniqueness [8]. To study the technical details and the precise definitions, we refer to [8,9]. Moreover, the findings of Dehmer et al. [8] revealed that the uniqueness of $J$ by using exhaustively generated graphs is poor. For example by using the class $N_{10}$ (all non-isomorphic graphs with 10 vertices), $|N_{10}| = 11,716,571,$ the
Balaban index $J$ could only discriminate 20% of $N_{10}$ uniquely. Nevertheless, $J$ has high uniqueness for alkane trees and isomers [9,13].

To define $j$, we require the definition of $D_{\text{MAX}}$ [12]:

$$(D_{\text{MAX}})_{ij} = \begin{cases} (D)_{ij} & \text{if } (D)_{ij} \geq \min\{R,C\} \\ 0 & \text{if } (D)_{ij} < \min\{R,C\} \end{cases}$$

Following Randić et al., the topological index $j$ is just the $D_{\text{MAX}}$ analog to Balaban’s $J$ index, see [2]. Based on the fact that $j$ can discriminate the remaining isomers of $n$-dodecane and $D_{\text{MAX}}$ has often a different structure compared to $D$, Randić et al. concluded that $D_{\text{MAX}}$ and, hence, $j$ may be a promising tool for graph isomorphism testing, see [2]. In the next section, we see that this statement has been too premature when evaluating $j$ on general and exhaustively generated graphs. By evaluating characteristic properties (e.g., the uniqueness) of topological graph measures on such (general) graphs, one can conclude how the index behave in the context of using complex networks.

### Results

Before interpreting Table 1, we explain its notation. We here used the graph classes $N_i$, $i=9,10$ [8] and $C_i$, $19\leq i \leq 22$ [8]. Again $N_i$ is the class of all exhaustively generated non-isomorphic and connected graphs with $i$ vertices [8]. $C_i$ is the class of exhaustively generated non-isomorphic and connected alkane trees [8]. $\text{ndv}$ stands for the number of non-distinguishable values [8] and $S = \frac{|G| - \text{ndv}}{|G|}$ where $G$ is a class of graphs, see [7].

Table 1 shows numerical results when comparing $j$ and $J$ on the just explained graph classes. We observe that the uniqueness of $j$ is quite poor for all graph classes. In case of using $N_9$, the uniqueness of $j$ is approximately as low as the uniqueness of $J$. That means both topological indices can only discriminate about 39% out of 261080 graphs. By considering the results for $J$, we see that $J$ possesses high uniqueness when using $C_i$. Note that this has already been found by Balaban [13] and Dehmer et al. [8]. But it is surprising that the uniqueness of $j$ is, without exception, much worse than the one of $J$. Table 2 shows that $j$ can discriminate the isomers of $n$-dodecane for which the Balaban $J$ index is pairwisely degenerated.

A hypothesis is that the sparseness of $D_{\text{MAX}}$ leads to this effect described above. So this matrix can not capture the complexity of the used graphs meaningfully and, thus, $j$ is degenerated for most of the graphs. This result shows the complexity of the problem to construct highly unique graph measures on general and exhaustively generated graphs.

### Summary and Conclusion

This paper investigated the uniqueness of the recently developed topological index $j$ introduced by Randić et al. [2]. $j$ has been defined quite similarly as it is based on the novel matrix $D_{\text{MAX}}$ instead of $D$. Based on small tests and by only using example graphs, Randić et al. [2] hypothesized $j$ has higher uniqueness than $J$ and, the index $j$ which combined with index $J$, may suffice to resolve the graph isomorphism issue for most cases of molecular graphs.

In this paper we have evaluated this hypothesis on a large scale by using general graphs. In fact, our study disproved this conjecture and demonstrated that the uniqueness of $j$ is quite poor by using general exhaustively generated graphs and alkane trees. As future work, we plan to determine so-called degeneracy classes analytically for performing a proper mathematical treatment of the problem. In any way, the search for highly discriminating graph invariants should be continued [8,9,13,16]. Following Randić et al. [2], such measures could be used as a prescreening method and would eliminate need for detailed and elaborate tests on large number of cases. Also, this fact has already been raised by Dehmer et al. [9] where they developed information-theoretic network measures with very low degeneracy on exhaustively generated graphs for graph isomorphism testing.

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#### Table 1. The uniqueness of $j$ and $J$ measured by ndv and $S$.

| Graph class | cardinality | ndv | $S$ |
|-------------|-------------|-----|-----|
| $N_9$       | 261080      | 165109 | 0.36759 |
| $N_{10}$    | 11716571    | 9476268 | 0.1912081 |
| $C_9$       | 148284      | 144041 | 0.028614 |
| $C_{10}$    | 366319      | 359177 | 0.019496 |
| $C_{11}$    | 910726      | 898838 | 0.013053 |
| $C_{12}$    | 2278658     | 2258804 | 0.00871302 |
| $J$         | 261080      | 156674 | 0.399900 |
| $N_{10}$    | 11716571    | 9307263 | 0.205633 |
| $C_9$       | 148284      | 5967 | 0.95975 |
| $C_{10}$    | 366319      | 44800 | 0.877702 |
| $C_{11}$    | 910726      | 45703 | 0.949816 |
| $C_{12}$    | 2278658     | 306911 | 0.865310 |

#### Table 2. The values of $J$ and $j$ by using the isomers of $n$-dodecane.

| Graph ID | $J$  | $j$  |
|----------|------|------|
| 1        | 4.252509 | 13.15875 |
| 2        | 4.252509 | 16.04085 |
| 3        | 3.752273 | 15.86058 |
| 4        | 3.752273 | 11.99851 |
| 5        | 4.135003 | 15.04953 |
| 6        | 4.135003 | 11.07033 |
| 7        | 3.575256 | 13.16886 |
| 8        | 3.575256 | 11.81169 |
| 9        | 3.773441 | 21.73837 |
| 10       | 3.773441 | 7.43385 |
| 11       | 3.954123 | 12.76649 |
| 12       | 3.954123 | 10.84469 |
Author Contributions
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