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Structural Differentiation of Graphs Using Hosoya-Based Indices

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Abstract

In this paper, we introduce the Hosoya-Spectral indices and the Hosoya information content of a graph. The first measure combines structural information captured by partial Hosoya polynomials and graph spectra. The latter is a graph entropy measure which is based on blocks consisting of vertices with the same partial Hosoya polynomial. We evaluate the discrimination power of these quantities by interpreting numerical results.

Introduction

Structural differentiation entails the classification of graphs according to structural features captured by quantitative measures, see, e.g., [1–5]. One way to demonstrate a classification procedure is to apply a measure (or index) to a special class of graphs and show that the measure discriminates between non-isomorphic graphs with high probability. A prominent example is the Balaban J index [6–8] which is highly discriminating on chemical graphs. However, this index has limitations as shown by Dehmer et al. [2] by means of a statistical analysis of the performance of the J and other indices on an exhaustively generated set of graphs without structural constraints, see [2]. This analysis shows that the discrimination power (also called uniqueness [2]) of graph measures depends on the underlying class of graphs [2].

This paper is an investigation of the discriminating power of structural indices based on the zeros of partial Hosoya polynomials and graph spectra. Also, we introduce and evaluate the Hosoya information content of a graph. To position this investigation we begin with a survey of literature dealing with eigenvalues and entropy-based measures of graphs. Classical results in the theory of graph spectra are due to Gutman et al. [9]. The main concern of this theory is to explore structural properties of graphs and complex networks captured by graph spectra [10]. More recent results have been presented and surveyed by Chung [11] and Cioabă [12]. Interdisciplinary applications of graph spectra, e.g., the analysis of biological networks and web graphs can be found in [10,13]. Various graph measures incorporating eigenvalues have been discussed by Randić et al. [14] and Dehmer et al. [15]. One example of a measure is defined as the sum of the moduli of non-zero eigenvalues of the adjacency matrix of a graph; another is given by graph entropies based on the eigenvalues of matrices associated with a graph [14–16]. Yet another well-known measure is the Estrada index [17–20] which has been explored in bioinformatics, mathematical chemistry and applied mathematics. A more recent review of this quantity is due to Gutman et al. [21]. Variants of these measures using other matrices have been discussed by Li et al. [22]. A related measure is the so-called energy of a graph which is an important quantity defined in relation to the eigenvalues of matrices associated with a graph, see [23–25]. Extremal properties of graph energy have been studied by [23–25]. A recent book on graph energy summarizing classical and new results is [26]. Inequalities for eigenvalue-based graph measures have been discussed in [12]. Elphick and Wocjan [27] analyzed a novel spectral measure for determining network irregularity [27].

Graph entropy measures have been explored extensively in various disciplines. Rashevsky and Mowshowitz did seminal work when developing the first graph entropy measures based on vertex orbits [28,29]. Korner introduced a graph entropy measure that has been used in information theory [30]. Bonchev et al. developed the magnitude-based information indices and various others based on graph invariants such as vertex degrees and distances in graphs [31–34]. Also, Bonchev et al. [1] proposed an information index for graphs which is based on the Hosoya graph decomposition. However, this information index (using Hosoya index Z [35] to define the probabilities of the induced partition) is quite different from the one we introduce here in section ‘Hosoya-based Indices’. Many other graph entropy measures can be found in [36–38]. To study results towards the Hosoya polynomial, we refer to [39,40].
...Hosoya polynomials, see [3]. As outlined in [3], the partial Hosoya
Hosoya-Spectral indices contribution of this paper is to define the
vertices

\[ d(v, v) = \min \{l(v, v) : v \neq v\} \]

where \( d(v, v) \) is the distance (i.e., length of a shortest path) between
the vertices \( v \) and \( v \). Solving the equation

\[ H^v(G, z) = 0, \]

yields the complex zeros \( z_{1}^{v}, z_{2}^{v}, \ldots, z_{k}^{v} \) which are not equal to
zero. We infer \( k < |V| \) by applying the well-known fundamental
theorem of Algebra [43,44] stating that a complex polynomial

\[ f(z) = a_{k}z^{k} + a_{k-1}z^{k-1} + \cdots + a_{1}z + a_{0}, a_{0} \neq 0, a_{k} \in \mathbb{C}, \]

with degree \( \deg(f) = k \) has \( k \) complex zeros.

Also in [3], Dehmer et al. introduced the following indices:

\[ M_1(G) = \left( |z_1^v| + |z_2^v| + \cdots + |z_{k-1}^v| \right) + \left( |z_1^{v'}| + |z_2^{v'}| + \cdots + |z_{k-1}^{v'}| \right) \]

\[ + \cdots + \left( |z_1^{v_k}| + |z_2^{v_k}| + \cdots + |z_{k-1}^{v_k}| \right) \]

\[ M_2(G) = \sqrt{|z_1^v| + |z_2^v| + \cdots + |z_{k-1}^v|} + \sqrt{|z_1^{v'}| + |z_2^{v'}| + \cdots + |z_{k-1}^{v'}|} \]

\[ + \cdots + \sqrt{|z_1^{v_k}| + |z_2^{v_k}| + \cdots + |z_{k-1}^{v_k}|} \]

...
measures special attention. In contrast to the previously introduced HS
More precisely, the discrimination power of the new measures can be explained by the fact that partial Hosoya polynomials and graph spectra capture quite different aspects of graph structure. In particular, the partial Hosoya polynomial captures local graph properties related to distances in a graph, and the indices $M_i$ take account of the moduli of the zeros of these polynomials. By contrast, the spectrum of a graph captures connectivity properties linked to its adjacency matrix. The combination of these graph properties in the measures $HS_i$ plausibly accounts for their superior performance over the single property measures $\langle M_i \rangle$.

Evidently, the discrimination power of $IH$ declines as the graph classes grow in size, i.e., the greater the cardinality of the graph class, the lower is index's discrimination power (measured by ndv and S), see Table 1–3. Even for small classes, the degeneracy is high. For $N_9$, the Hosoya information content $IH$ cannot discriminate at all and, hence, $S=0$. These results are not surprising in view of the definition of Hosoya information content. The blocks of the partitions consist of vertices with the same partial Hosoya polynomial. Thus, the more cycles in a graph, the greater the likelihood of obtaining large blocks of vertices with the same partial Hosoya polynomial. The occurrence of such large blocks results in high values for the quantity ndv and low values for $S$.

### Summary and Conclusions

In this paper, we defined the Hosoya-Spectral indices as well as the Hosoya information content of a graph. The former measures combine structural information captured by partial Hosoya polynomials and graph spectra. It is evident that those two graph features capture structural information differently and, hence, the resulting measures may be more unique than the ones $\langle M_i \rangle$ used in earlier work, see [3]. The numerical study reported here has confirmed this conjecture for both trees and graphs. Finally, as expected, the discrimination power of Hosoya information content was found to be very low.

In future research, we plan to explore extremal properties of both measures. In particular, Hosoya information content is
related to the orbit structure of a graph, and this calls for studying
the automorphism groups of certain classes of graphs.

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References

discriminative power for graphs. PLoS ONE 7: e31521.
measures based on complex zeros of the partial Hosoya polynomial. submitted for publication.
4. Konstantinova EV, Palev AA (1990) Sensitivity of topological indices of
perception of duplicated chemical structures in large chemical databases.
Application. Deutscher Verlag der Wissenschaften. Berlin, Germany.
Applications. Oxford University Press.
11. Chung F (1997) Spectral Graph Theory, volume 12 of
Cbms Regional
the automorphism groups of certain classes of graphs.
discussions
Randic M, Orel R, Balaban AT (2013) Entropy theory, distance matrix and
measures based on complex zeros of the partial Hosoya polynomial. submitted for publication.
Letters 319: 713–718.
25. Randić M (2013) Information Theoretic Indices for Characterization of
29. Mowshowitz A (1968) Entropy and the complexity of the graphs I: An index of
31. Bonchev D, Trinajstic N (1977) Information theory, distance matrix and
35. Deutsch E, Klavžar S (2013) Computing the hosoya polynomial of graphs from
37. Konstantinova EV, Skorobogatov VA, Vidyuk MV (2002) Applications of

Author Contributions

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