Abstract

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Information indices with high discriminative power for graphs

In this paper, we evaluate the uniqueness of several information-theoretic measures for graphs based on so-called information functionals and compare the results with other information indices and non-information-theoretic measures such as the well-known Balaban *J* index.

We show that, by employing an information functional based on degree-degree associations, the resulting information index outperforms the Balaban *J* index tremendously. These results have been obtained by using nearly 12 million exhaustively generated, non-isomorphic and unweighted graphs. Also, we obtain deeper insights on these and other topological descriptors when exploring their uniqueness by using exhaustively generated sets of alkane trees representing connected and acyclic graphs in which the degree of a vertex is at most four.