Abstract

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Novel topological descriptors for analyzing biological networks

Background: Topological descriptors, other graph measures, and in a broader sense, graph-theoretical methods, have been proven as powerful tools to perform biological network analysis. However, the majority of the developed descriptors and graph-theoretical methods does not have the ability to take vertex- and edge-labels into account, e.g., atom- and bond-types when considering molecular graphs. Indeed, this feature is important to characterize biological networks more meaningfully instead of only considering pure topological information.

Results: In this paper, we put the emphasis on analyzing a special type of biological networks, namely biochemical structures. First, we derive entropic measures to calculate the information content of vertex- and edge-labeled graphs and investigate some useful properties thereof. Second, we apply the mentioned measures combined with other well-known descriptors to supervised machine learning methods for predicting Ames mutagenicity. Moreover, we investigate the influence of our topological descriptors - measures for only unlabeled vs. measures for labeled graphs - on the prediction performance of the underlying graph classification problem.

Conclusions: Our study demonstrates that the application of entropic measures to molecules representing graphs is useful to characterize such structures meaningfully. For instance, we have found that if one extends the measures for determining the structural information content of unlabeled graphs to labeled graphs, the uniqueness of the resulting indices is higher. Because measures to structurally characterize labeled graphs are clearly underrepresented so far, the further development of such methods might be valuable and fruitful for solving problems within biological network analysis.