Abstract

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A comparative analysis of the Tanimoto index and graph edit distance for measuring the topological similarity of trees.

In this paper we explore interrelations between the Tanimoto index and the graph edit distance (GED) for measuring the topological similarity/distance of graphs.

To do so, we discuss cumulative similarity/distance distributions of these measures and other data analysis methods.

Also we explore properties of the Tanimoto index by using sets of chemical alkane trees and exhaustively generated ordinary trees as subgraphs.

In particular, we discuss numerical results for exploring the approximation behavior of the Tanimoto index by GED.