Parallel Branch-and Bound Approach with MPI Technology in Inferring Chemical Compounds with Path Frequency

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Abstract

Drug design is the approach of finding drugs by design using computational tools. When designing a new drug, the structure of the drug molecule can be modeled by classification of potential chemical compounds. Kernel Methods have been successfully used in classifying potential chemical compounds. Frequency of labeled paths has been proposed to map compounds into feature in order to classify the characteristics of target compounds. In this study, we proposed an algorithm based on Kernel method via parallel computing technology to reduce compute time. This less constrain of timing allows us to aim at back tracking a full scheme of all of the possible pre-images, regardless of their difference in molecular structure, only if they shared with the same feature vector. Our method is modified on BB-CIPF. To reduce the computing time, the method we proposed used MPI to solve the computing time issue. The experimental results show that our algorithms can reduce the computation time for chemical compound inference problem.

Keyword：chemical compound inference, parallel branch-and-bound, MPI