

Efficient parallel branch-and-bound algorithm for constructing minimum ultrametric trees

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Abstract

Constructing evolutionary trees is an important problem in the computational biology and in the taxonomy. The ultrametric tree (UT) is a commonly used model for evolutionary trees which is assumed that the rate of evolution is constant (molecular clock hypothesis). However, it has been shown to be NP-hard to construct minimum ultrametric trees (MUTs) (principle of minimum evolution) even from a metric distance matrix. The branch-and-bound is generally used algorithm to solve a wide variety of NP-hard problems. In our previous work, a sequential branch-and-bound algorithm for constructing MUTs (BBU) was presented and the experimental results showed that the branch-and-bound algorithm is useful for MUTs construction problem. Hence, in this paper, we design an efficient parallel branch-and-bound algorithm (PBBU) for constructing MUTs or near-MUTs from a metric distance matrix. A random data set and practical data sets of Human+Chimpanzee Mitochondrial and bacteriophage T7 DNAs are used to test PBBU. The experimental results show that the PBBU can find an optimal solution for 36 species within a reasonable time on 16 PCs, to the best of our knowledge, there is no report of algorithms solving this problem even for 25 species. Moreover, the PBBU can achieve satisfied speed-up ratios for most of testing cases.

Keyword : Parallel branch-and-bound algorithm, Evolutionary tree construction, Distance matrix, Minimum ultrametric tree, Load-balancing