NEW ALGORITHM FOR THE MAXIMUM CLIQUE PROBLEM

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A new algorithm for finding a maximum clique in an undirected graph is described. An approximate coloring algorithm has been improved and used to provide bounds to the size of the maximum clique in a basic algorithm which finds a maximum clique. This basic algorithm was then extended to include dynamically varying bounds. The resulting algorithm is significantly faster than the comparable algorithm. This algorithm is used for comparing protein structures, to provide the information about protein function and also the information about possible interactions between proteins. The principles of graph theory are adopted to investigate protein structures and predicting protein binding sites.

Keywords: maximum clique algorithm, graph coloring, probis web-server.
AMS Subject Classification: 68R10, 05C15, 05C85.

References

[1] J. Konc, D. Janežič, An improved branch and bound algorithm for the maximum clique problem, MATCH Commun. Math. Comput. Chem. 58 (2007) 569-590.

[2] J. Konc, D. Janežič, ProBiS algorithm for detection of structurally similar protein binding sites by local structural alignment, Bioinformatics 26 (2010) 1160-1168.

[3] J. Konc, D. Janežič, ProBiS: a web server for detection of structurally similar protein binding sites, Nucleic Acids Research 38 (2010) W436-W440.