

论文

改进的自组织映射(SOM)蛋白质折叠算法和计算实现

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摘要 蛋白质结构预测是生物信息学中的重要研究方向. 为了研究蛋白质折叠的机理, 人们引入了

只考虑蛋白质疏水核心和亲水外围位置导致能量差别的简化~HP~模型. 即使是求解二维~HP~模型已被

证明是一个~NP~完全问题, 因此需要设计有效的近似算法来求解较大规模的~HP~模型. 从旅行商问

题~(TSP)~的求解看, 自组织映射是构造近似算法的有效工具. 本文将归一化的~F-W~自组织模型应用

到蛋白质二维~HP~问题的求解中, 结合为克服多重映射构造的局部线搜索算法. 数值试验表明, 该

算法改进了现有的~HP~模型的~SOM~求解算法, 只需很少的迭代步数就能找到最低能量构象. 这一

改进算法可以成为进一步研究的基础.

关键词 [蛋白质折叠](#) [结构预测](#) [自组织映射](#) [HP模型](#)

分类号

IMPROVED SELF-ORGANIZING MAP ALGORITHM FOR PROTEIN FOLDING AND ITS REALIZATION

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Abstract Protein structure prediction is one of the main research topics in bioinformatics. A simple exact HP model is introduced in order to go deep into the principles of the protein folding, which only considers the energy difference caused by the hydrophobic core and polar periphery. It has been proved that this problem is NP-complete and the right way is looking for approximate solution. In this paper a normalized F-W SOM algorithm is constructed for the two dimensional HP model of protein folding, inspired by the efficient behavior of SOM in solving the classical Traveling Salesman Problem (TSP). Also a local search method is designed to overcome the multi-mapping phenomenon. Numerical results show that this algorithm improves the existed SOM algorithm for HP model and can find the minimum energy configuration in less iterations.

Key words [Protein folding](#) [protein structure prediction](#) [self-organizing map](#) [HP model](#)

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