

Semi-parameter Adaptation Information Assisted Multi-objective Differential Evolution for Protein-ligand Docking

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For the protein-ligand molecular docking optimization problem, a novel semi-parameter adaptive information-assisted multi-objective differential evolution method, named SAIAM, is proposed. To comprehensively consider the connectivity and dimension of the ligand flexibility during the docking optimization, SAIAM employs a stage-wise and dynamic semi-parameter adaptive strategy. In the previous stage of the search process, the crossover rate is randomly generated from the normal distribution and updated adaptively using the weighted arithmetic average algorithm, thus maintaining the diversity of the population. In the latter stage of the search, the scaling factor is generated by the Cauchy distribution and updated using the Lehmer mean, which enhances the global exploration and local exploitation capabilities of the system. Additionally, SAIAM introduces the AdaInf algorithm to update the weights in gradient descent using an infinity-norm-based rule, which can smooth the learning rate decay and enhance the handling of the large outliers, and improve the convergence of the algorithm to explore the global optimal solutions. Furthermore, SAIAM proposes a population size strategy based on the combination of the linear and sawtooth functions, effectively improving its execution efficiency. The experimental results demonstrate that the proposed SAIAM has excellent performance in terms of the accuracy and execution efficiency of the conformation search for protein-ligand docking, indicating its strong global and local development capabilities.

References:

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