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Title: Automated Design of Hyper-Heuristics Components to Solve the PSP Problem with HP Model
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Abstract:
The Protein Structure Prediction (PSP) problem is one of the modern most challenging problems from science. Simplified protein models are usually applied to simulate and study some characteristics of the protein folding process. Hence, many heuristic strategies have been applied in order to find simplified protein structures in which the protein configuration has the minimal energy. However, these strategies have difficulties in finding the optimal solutions to the longer sequences of aminoacids, due to the complexity of the problem and the huge amount of local optima. Hyper heuristics have proved to be useful in this type of context since they try to combine different heuristics strengths into a single framework. However, there is lack of work addressing the automated design of hyper-heuristics components. This paper proposes GEHyPSP, an approach which aims to achieve generation, through grammatical evolution, of selection mechanisms and acceptance criteria for a hyperheuristic framework applied to PSP problem. We investigate the strengths and weaknesses of our approach on a benchmark of simplified protein models. GEHyPSP was able to reach the best known results for 7 instances from 11 that composed the benchmark set used to evaluate the approach.

Preferred form of presentation: Oral

Paper Topics:
SS24. Evolutionary Computation in Bioinformatics
1k. Heuristics, metaheuristics and hyper-heuristics
SS01. Evolutionary Computation for Automated Algorithm Design

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Sincerely,
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