Parallel Algorithm Portfolios with Adaptive Resource-Allocation Strategy

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Extended Abstract

Algorithm portfolios [1, 2] have gained increasing popularity as general multi-algorithm frameworks for global optimization. The rationale behind their development lies in the fact that, given a previously unknown problem, it is preferable to apply an algorithmic scheme that combines multiple algorithms (or their variants) running interchangeably or concurrently, instead of a single algorithm selected arbitrarily from the relevant literature. Thus, the user is relieved from the burden of selecting an appropriate algorithm, which commonly comes at the risk of a poor choice, especially in cases where there is no adequate *a priori* information on the specific problem. Also, the problem of parameter setting of the selected algorithm is alleviated since the user can include different variants of a specific algorithm in the algorithm portfolio.

In algorithm portfolios, the available computational resources, i.e., function evaluations (also referred as the computation budget) or available processing units, are gradually allocated in episodes (a.k.a. batches) to the constituent algorithms, each one assigned only a fraction of the available resources at each time. In the case of serial execution on a single processing unit, each constituent algorithm is assigned a fraction of the computation budget at each episode, and it consumes it before proceeding to the next algorithm, in a round-robin manner. In the case of parallel execution in multi-processor environments, each constituent algorithm can occupy one processing unit while sharing the available computation budget with the rest as in the serial case. Alternatively, it can occupy multiple processing units each, spending a fixed computation budget per processing unit at each episode.

It is easily perceived that the resource-allocation procedure plays primary role in the efficiency of an algorithm portfolio. Offline resources allocation prior to execution may result in sub-optimal performance of the portfolio. On the other hand, an online allocation procedure can capture the relative performance

of each algorithm at the different stages of the optimization procedure and allocate the resources, accordingly. This way, the most efficient algorithms are awarded additional resources, while the less efficient ones are not neglected since they may be useful in later stages (e.g., exploration-oriented vs exploitation-oriented algorithms). Relevant works verified these properties using various resource allocation schemes [2].

The present work proposes a resource allocation scheme based on adaptive decision-making procedures. More specifically, a parallel algorithm portfolio consisting of three state-of-the-art optimization algorithms is considered. The constituent algorithms are (i) the BFGS quasi-Newton method, (ii) the nonlinear simplex method of Nelder and Mead, and (iii) the population-based particle swarm optimization method. The selected algorithms belong to the three essential categories of numerical optimization algorithms, namely gradient-based, direct search, and evolutionary algorithms, respectively. To the best of our knowledge, this is the first algorithm portfolio in literature that combines algorithms from all these categories. Each algorithm occupies a processing unit (worker) in a master-worker parallel computation model. The computation budget (function evaluations) is allocated in episodes to the three algorithms.

While the first assignment is fair among the algorithms, their performance is assessed in terms of solution quality according to an adaptive pursuit strategy after each episode. The specific adaptive decision-making approach was selected based on its tolerance in non-stationary environments and its previous performance in relevant resource allocation tasks [3]. Thus, after each episode, each algorithm is assigned a reward and its forthcoming allocated budget is determined according to the reward as well as an estimation of its future quality, similarly to a reinforcement-learning approach.

The proposed scheme is benchmarked on a challenging and computationally demanding problem, namely the problem of atoms configuration through the minimization of Lennard-Jones potentials. The specific problem exhibits high number of local minima and scales exponentially with the number of atoms. Experimental results on various molecules ranging from 20 to 80 atoms reveal that the algorithm portfolio outperforms all its constituent algorithms on the specific problems. Also, different configurations of the algorithm portfolio are studied and analyzed. The results are supported by complete statistical analysis, providing insight on the proposed algorithmic schemes.

References

[1] B. A. Huberman, R. M. Lukose, and T. Hogg. An economics approach to hard computational problems. *Science*, 27:51–53, 1997.

[2] D. Souravlias, K.E. Parsopoulos, I.S. Kotsireas, and P.M. Pardalos. *Algorithm Portfolios: Advances, Applications, and Challenges*. SpringerBriefs in Optimization. Springer, 2021.

[3] D. Thierens. An adaptive pursuit strategy for allocating operator probabilities. In *Proceeding of the GECCO 2005 Conference (Washington, DC, USA)*, pages 1539–1546. ACM, 2005.