Understanding Exploration and Exploitation Powers of Meta-heuristic Stochastic Optimization Algorithms through Statistical Analysis

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ABSTRACT

Understanding of exploration and exploitation powers of meta-heuristic stochastic optimization algorithms is very important for algorithm developers. For this reason, we have recently proposed an approach for making a statistical comparison of meta-heuristic stochastic optimization algorithms according to the distribution of the solutions in the search space, which is also presented in this paper. Its main contribution is the support to identify exploration and exploitation powers of the compared algorithms. This is especially important when dealing with multimodal search spaces, which consist of many local optima with similar values, and large-scale continuous optimization problems, where it is hard to understand the reasons for the differences in performances. Experimental results showed that our recently proposed approach gives very promising results.

CCS CONCEPTS

• **Mathematics of computing → Hypothesis testing and confidence interval computation**;

KEYWORDS

Statistical analysis, stochastic optimization algorithms

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1 INTRODUCTION

Information that is covered by the distribution of the obtained solutions in the search space can be used for better understanding of the exploration and exploitation powers of stochastic optimization algorithms. By performing comparison of the algorithms with regard to the obtained solutions values and their distribution in the search space, we can distinguish between four scenarios:

- There is no statistical significance between the algorithms according to the obtained solutions values and their distribution. This indicates that the compared algorithms have the same exploration and exploitation power.
- There is no statistical significance between the performances of the compared algorithms with regard to the obtained solutions values, but there is a statistical significance with respect to the distribution of the obtained solutions in the search space. This indicates that the algorithm with the sparser distribution of obtained solutions has better exploration power.
- There is a statistical significance between the compared algorithms with regard to the obtained solutions values, but there is no statistical significance as to the distribution of the obtained solutions in the search space. This indicates that the compared algorithms are able to find a region with good solutions (have the same exploration power), but one is able to find statistically better solutions than the other in the same region (have different exploitation powers). Such kind of analysis show that the "losing" algorithm must improve its exploitation power.
- There is a statistical significance between the algorithms according to the obtained solutions values and their distribution. This indicates that the poorer performing algorithm lacks exploration power, while its exploitation power cannot be assessed and therefore, first, the exploration power needs to be improved.

Such analyses can be helpful in understanding what the optimization algorithm lacks. For this reason, we recently proposed the extended Deep Statistical Comparison approach that provides information on the exploration and exploitation powers of the compared algorithms [1].

2 EXTENDED DEEP STATISTICAL COMPARISON

To the best of our knowledge, there are no published papers in which statistical analyses of stochastic optimization algorithms

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according to the distribution of the obtained solutions in the search space are presented. This kind of analysis is extremely welcome because it can further provide a deeper understanding of the methodologies used to improve the exploration and exploitation powers of the optimization algorithms.

The extended Deep Statistical Comparison (eDSC) is a generalization of the Deep Statistical Comparison (DSC) [2]. It involves two steps. The first step uses the DSC ranking scheme to compare the algorithms with regard to the obtained solutions values. In addition to this, it introduces a novel eDSC ranking scheme that compares algorithms with regard to the distribution of the solutions in the search space.

The eDSC ranking scheme follows the same idea as the DSC ranking scheme (i.e. comparing distributions). However, in the case of eDSC, the mathematics is completely different because high-dimensional data is involved in the comparison instead of one-dimensional data used by the DSC ranking scheme. For each problem (i.e. function) on which the selected algorithms are compared, the eDSC ranking scheme preforms all pairwise comparisons by comparing their distributions using the multivariate ϵ test. Further, the obtained p-values are organized in a matrix and because multiple pairwise comparisons are made, they are corrected using the Bonferroni correction. There is also a theoretical explanation that shows that the distributions of the obtained solutions, $\mathbf{x_1}, \ldots, \mathbf{x_{n_1}}$ and $\mathbf{x'_1}, \ldots, \mathbf{x'_{n_2}}$, between two algorithms are statistically significant when the subtraction of the sum of both within distances of the solutions from the between distance of the solutions (see Equation 1) should be greater than a critical value, which can be calculated from a degenerate two-sample V-statistic for a given significance level α.

$$\mathcal{E}_{n_1,n_2} = \frac{n_1 n_2}{n_1 + n_2}\left(\frac{2}{n_1 n_2}\sum_{i=1}^{n_1}\sum_{j=1}^{n_2}||\mathbf{x_i} - \mathbf{x'_j}|| - \frac{1}{n_1^2}\sum_{i=1}^{n_1}\sum_{j=1}^{n_1}||\mathbf{x_i} - \mathbf{x_j}|| - \frac{1}{n_2^2}\sum_{l=1}^{n_2}\sum_{j=1}^{n_2}||\mathbf{x'_l} - \mathbf{x'_j}||\right). \quad (1)$$

Next, the key point for the ranking scheme is checking the p-value matrix transitivity.

If the transitivity is satisfied, it means that the distributions of the obtained solutions in the search space are not statistically significant and all algorithms should obtained the same ranking.

If the transitivity is not satisfied, the user should first define the spread preference of the solutions in the search space. After that, the square root of the determinant of the solutions covariance matrix for each algorithm is used as a measure for multivariate spread. With this the hypervolume is introduced, incorporating both shape (correlation) and size (standard deviation) information, which is the product of the standard deviations of the principal components. The hypervolume covered by the distribution of the solutions in the search space for each algorithm can be calculated as a product of the eigenvalues that are obtained from eigenvalue decomposition of its covariance matrix. However, it can happen that the covariance matrix is not a positive-definite because it is singular, which means that at least one of the variables can be expressed as a linear combination of the others. In this case, before calculating the eigenvalues needed for the hypervolume, dimensionality reduction should be applied to reduce the number of variables under consideration, by obtaining a set of principal variables, or by computing the nearest positive-definite matrix to an approximate one. Once the hypervolumes of the compared algorithms are calculated, they are ranked according to the selected user preference.

After obtaining the eDSC rankings for each problem involved in the benchmark data set, they are further used as an input data for second step, which consists of an appropriate omnibus statistical test in order to perform the benchmarking.

3 DISCUSSION

Experimental results obtained using the results from the Black-Box Benchmarking 2009 competition showed that the novel proposed approach can give deeper understanding of exploration and exploitation powers of the compared algorithms.

Large-scale continuous optimization, which is currently one of the most active research areas in optimization, could also benefit of such kind of analysis. In large-scale dimensional problems, compared to low-dimensional problems, it is even harder to understand the reasons for the differences in performances of the compared algorithms, due to enormous sizes and complexities of hundred or even thousand dimensional search spaces.

The eDSC approach can also be used to estimate how the search ability of the algorithms depends on either their initial conditions or on the parameters. For this purpose, we can take one algorithm with different initial conditions or different parameters and treat each instance as a different algorithm.

4 CONCLUSION

When dealing with stochastic optimization algorithms, information about the distribution of solutions in the search space can be helpful for understanding the exploration and exploitation powers of the algorithms. For this reason, we presented a recently proposed approach for making a statistical comparison of meta-heuristic stochastic optimization algorithms according to solution values and distribution of the solutions in the search space, which provides deeper understanding of the exploration and exploitation powers of the compared algorithms.

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