Bridging Kriging Believer and Expected Improvement Using Bump Hunting for Expensive Black-box Optimization

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ABSTRACT

For several real-world optimization problems, the evaluation of response functions may be expensive, computationally or otherwise. The number of design evaluations one can afford for such problems are therefore severely limited. Surrogate models are commonly used to guide the search for such computationally expensive optimization problems (CEOP). The surrogate models built using a limited number of true evaluations are used to identify the next *infill/sampling* location. Expected improvement (EI) is a well known infill criteria which balances exploration and exploitation by accounting for both mean and uncertainties in the current model. However, recent studies have shown that, somewhat counter-intuitively, a greedy ("believer") strategy can compete well with EI in solving CEOPs. In this study, we are interested in examining the relative performance of the two infill methods across a range of problems, and identify the influencing factors affecting their performance. Based on the empirical analysis, we further propose an algorithm incorporating the strengths of the two strategies. The numerical experiments demonstrate that the proposed algorithm is able to achieve a competitive performance across a range of problems with diverse characteristics; making it a strong candidate for solving black-box CEOPs.

KEYWORDS

Kriging believer, Expected improvement, Hybrid optimization

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1 INTRODUCTION

Surrogate assisted optimization (SAO) is commonly adopted for solving CEOPs. A widely used infill criterion is expected improvement (EI) maximization. Its advantage lies in overcoming local optimum and global convergence. However, recent studies, including [4] show that, counter-intuitively, Kriging believer (KB) infill criterion can outperform EI strategy in certain scenarios. In this paper, we conduct numerical experiments on problems with diverse features in a controlled setting to provide further insights on the relative performance of KB and EI. Based on the above analysis, we propose a hybrid optimization algorithm that can act as a bridge between the conventional KB and EI infill criteria and combine their strengths. The key aim is to generate competitive (though not necessarily the best) performance across problems with different features without prior knowledge of modality, so that the algorithm can be more confidently applied to unseen cases.

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2 MOTIVATING OBSERVATIONS

As mentioned previously, KB has shown competitive performance even for some multimodal problems [4]. By comparing the principles of these two strategies, we infer that global structure of the objective landscape could be one of the major factors that offer advantages to the KB strategy. The presence of a global structure refers to the functions where optimum of the low-fidelity models based on relatively sparse sampling lies close to the global optimum, a representative example being the Rastrigin function. In such landscapes, even with multimodality, KB still can quickly locate global optimum. However, without the presence of global structure, KB can get stuck in local optimum, while EI is able to perform better on account of its relatively higher tendency to sample in uncertain regions to improve the global model, for example in the case of Shekel function. In order to combine the strengths of these two infill criteria, we intend to identify promising regions based on currently evaluated solutions, and would like to supplement the EI search by additional, concentrated sampling using KB in these regions. We propose to identify these promising regions approximately using a data analysis technique called *bump hunting* [2].

3 PROPOSED APPROACH

The pseudo-code of the proposed algorithm, referred to as bump hunting assisted expected improvement based optimizer (BHEI), is presented in Algo. 1. BHEI for the most part operates on EI strategy, but incorporates a localized KB sampling periodically to overcome its above-mentioned shortcomings compared to KB. We set a frequency parameter δ to control the activation of local search. Every δ iterations, the local search is invoked to identify a promising region R^L with BH. BH extracts a series of candidate boxes from A, which stores all truly evaluated solutions. These boxes follow ascending order in terms of the average f value of enclosed points. To construct the local region, we start from the first box as a base local region, and increasingly add more boxes until the number of enclosed points reaches $2(d+1)$, including the current best solution in A. Within this promising region R^L, KB infill search is conducted to identify the local minimum point $\mathbf{x}^k_{infill}$ and its true objective

Algorithm 1 The proposed BHEI algorithm

Input: Max. number of function evaluations FE_{max}, Initial sample size n, frequency parameter δ, design variable dimensionality d
Output: Best solution $\mathbf{x}^*$ and f^*

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Sample n instances of x as x_n
Obtain their corresponding f_n values through true evaluations
Build kriging model D that maps x to f with GP.
Initialize archives A ← {x_n, f_n}, Update FE
while (FE < FE_max) do
    Use EI criterion to search for a next infill point x^e_infill
    Evaluate x^e_infill to obtain f^e_infill and update archives
    A ← {x^e_infill, f^e_infill} and FE
    Filter out close solutions from A based on ε
    if ((FE − n) mod δ) == 0 then
        Apply BH on A
        Identify best solution x^min_arc from A
        Increasingly merge BH returned boxes, till both x^min_arc
            is included and enclosed point size is greater than or
            equal to 2(d + 1)
        Extract training points from A within above
            identified local region R_local
        Build a local surrogate D_local.
        Apply KB infill search on D_local bounded by R_local
            identify an infill point x^k_infill
        Evaluate x^k_infill to get f^k_infill
        Update archive A ← {x^k_infill, f^k_infill} and FE
        Filter out close solutions from A based on ε
    end if
    Update kriging model D with archive A
end while
Report the best solution x* and f* from A
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value f^k_{infill}. When evaluation budget is exhausted, best solution in A is returned. An ill-conditioning check is done on A while adding any new truly evaluated solution using a tolerance $\epsilon = 1e-6$.

4 NUMERICAL EXPERIMENTS

For experiments, we select 16 problems with different features. The number of initial samples generated using latin hypercube sampling are set as $11 \times d - 1$, where $d = 3$ is the number of design variables. Total budget for evaluation is set to 200. Table 1 lists the results of median runs of three different algorithms. The symbols U and M refer to unimodal and multimodal, respectively. s and w refers to strong and weak modality, respectively, while sG and wG refer to strong and weak global structure, respectively. The symbols ↓, ↑ and ≈ refer to the former algorithm performs significantly worse, better or equivalent compared to the latter algorithm.

In the EI *vs* KB column (middle column), it can be seen that for unimodal problems, KB performs either significantly better or similar to EI. For multimodal problems, there are mixed results, with a subset where KB outperforms EI and vice-versa. These empirical results clearly show that KB and EI have their niches and outperform each other on different sets. The median results using BHEI, as well as the statistical significance tests w.r.t. KB and EI are summarized in the first and third columns. It can be seen that BHEI shows the best overall performance among the three algorithms. It performs better or equal to EI for 9 and 7 instances, respectively, while compared to KB the numbers are 7 and 8, respectively. It can be inferred that BHEI is a more reliable algorithm than either KB and EI.

Problem	Features	KB (*vs* BHEI)	EI (*vs* KB)	BHEI (*vs* EI)
1. SMD1L [5]	U	0.7264 ↓	0.5987≈	0.0099 ↑
2. SMD2L [5]	U	0.0005 ≈	0.0396 ↓	0.0011 ↑
3. Rosenbrock [6]	U	4.9507≈	12.6930 ↓	3.5501 ↑
4. Zakharov [6]	U	6.6152 ↓	5.6808≈	0.2716 ↑
5. Levy [6]	M (s, sG)	0.0109 ≈	0.2083↓	0.0032 ↑
6. Ackley [6]	M (s, sG)	0.0541 ↓	0.1771↓	0.0185 ↑
7. SMD3L [5]	M (w, sG)	1.7907↓	2.743≈	0.9618 ↑
8. SMD4L [5]	M (w, sG)	0 ↑	0.5168↓	0.0000 ↑
9. DSm [1]	M (w, sG)	0.1094 ≈	0.2329 ≈	0.0735 ↑
10. TP7 [3]	M (w, wG)	-2.0430≈	-2.5343 ≈	-2.2724 ≈
11. Shekel [6]	M (s, wG)	-3.0542↓	-10.7160↑	-10.5560≈
12. TP9 [3]	M (w, wG)	-3.6336 ≈	-4.3538 ≈	-4.3568≈
13.TP3 [3]	M (s, wG)	-2.6326 ≈	-2.8233 ≈	-2.7144 ≈
14. TP6 [3]	M (s, wG)	-3.4708↓	-3.7886 ≈	-3.9918 ≈
15. Rastrigin [6]	M (s, sG)	4.9748↓	2.0182 ↑	2.0132 ≈
16. TP5 [3]	M (s, sG)	-1.6000 ≈	-1.6940 ↑	-1.6587≈

Table 1: Test problems and results.

5 CONCLUSION AND FUTURE WORK

In this paper, we analyzed KB's competitive performance despite theoretical advantages of EI, particularly underlying problem features that result in these observations. We then proposed a hybrid algorithm BHEI that combines the strengths of KB and EI. Experimental results on a range of problems show that the proposed BHEI has competitive and reliable performance across diverse problem characteristics.

APPENDIX

DSm problem is modified from the lower level DS test problem [1].

$$\min f(\mathbf{x}) = \sum_{i=1}^{k} \mathbf{x}_i^2 + \sum_{i=2}^{k} 10 \times |\sin(\frac{\pi}{k} x_i)|; -k \le \mathbf{x}_i \le k, i \in \{1, ..., k\} \tag{1}$$

The SMD problems used in this study are bilevel problems [5]. We only use their lower level problems. For all four SMD problems, their upper level variable $\mathbf{x}_u$ is fixed to be $\mathbf{x}_u = [0, 0]$.

REFERENCES

[1] K. Deb and A. Sinha. 2009. Constructing test problems for bilevel evolutionary multi-objective optimization. In *IEEE Congress on Evolutionary Computation*. 1153–1160.

[2] Jerome H Friedman and Nicholas I Fisher. 1999. Bump hunting in high-dimensional data. *Statistics and Computing* 9, 2 (1999), 123–143.

[3] Ingo Paenke, Jurgen Branke, and Yaochu Jin. 2006. Efficient Search for Robust Solutions by Means of Evolutionary Algorithms and Fitness Approximation. *IEEE transactions on evolutionary computation* 10, 4 (2006), 405–420.

[4] Frederik Rehbach, Martin Zaefferer, Boris Naujoks, and Thomas Bartz-Beielstein. 2020. Expected Improvement versus Predicted Value in Surrogate-Based Optimization. In *Genetic and Evolutionary Computation Conference (GECCO)*.

[5] Ankur Sinha, Pekka Malo, and Kalyanmoy Deb. 2014. Test problem construction for single-objective bilevel optimization. *Evolutionary computation* 22, 3 (2014), 439–477.

[6] Sonja Surjanovic and Derek Bingham. 2013. Virtual Library of Simulation Experiments: Test Functions and Datasets. *Retrieved January 11, 2021, from http://www.sfu.ca/~ssurjano* (2013).