Ph.D. Thesis Review

Ph.D. candidate:Ing. Zbyněk Pitra, CTU in Prague, Fac. of Nuclear Sciences and Physical Eng.Thesis title:Surrogate Modeling and Landscape Analysis for Evol. Black-Box OptimizationExaminer:Petr Pošík, Ph.D.CTU in Prague, Fac. of Electrical Engineering, Dept. of Cybernetics

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The submitted Ph.D. thesis deals with the use of Gaussian processes as surrogate models in a particular type of evolutionary strategy, CMA-ES. The goal of using surrogate models in EAs is to improve their efficiency, i.e., to decrease the number of objective function evaluations required to find a solution with acceptable quality. This would greatly improve the applicability of such EAs in scenarios where evaluating the solution is costly or time-expensive. Such methods are currently studied very intensively. **The topic** of the thesis is thus **important**, **and interesting** for the community.

From the formal point of view, **the submitted work fulfills the usual conventions of scientific writing**. The thesis is written in a very good and readable English, with only a few typos. The main text of the thesis spans almost 170 pages and cites ca 200 works.

The thesis has a logical structure. After an introduction and description of the necessary background, the main work of the candidate is described in chapters 4 and 5. Chapter 4 presents a wellthought sequence of thorough investigations studying various aspects of the application of Gaussian processes and random forests as surrogate models in CMA-ES algorithm. This chapter presents a lot of interesting findings, e.g., that the type of a surrogate model and the way it is employed in an algorithm should not be assessed in isolation. Chapter 5 then presents interesting and valuable results of studies aimed at the usage of landscape analysis in surrogate model-assisted CMA-ES. Chapter 6 then summarizes the work, lists the author's contributions and suggests topics for future work.

Most of the sections in **these chapters are based on articles published by the author**. His publication record is good: besides ca 10 workshop publications, the candidate published his findings in 5 conference papers and at least one journal paper (another one is probably submitted, preprint can be found on arxiv). According to Google Scholar, his articles attracted over 200 citations which results in H-index 7.

From my point of view, the thesis contains the following main original contributions:

- a detailed experimental study of various facets of applying surrogate modeling in the CMA-ES algorithm;
- a successful application of Gaussian processes as a surrogate model in special version of CMA-ES which provides very competitive results;
- an experimental investigation of relations between landscape features and the performance of the CMA-ES algorithm with various surrogate models.

It should be emphasized that at least some of the results presented in this thesis are provably on par or beyond the current state of the art as examplified by the DTS-CMA-ES algorithm winning the Black-box optimization competition at the GECCO conference in 2017. In my opinion, **all the above contributions helped to advance the field of black-box optimization with surrogate models**.

To summarize, the thesis shows that **the Ph.D. candidate is able to systematically and indepen-dently perform research** in the chosen scientific area, and shows a good potential for further work in research. The results presented in this thesis are original and pushed the boundaries of knowledge in the area of surrogate modeling in evolutionary algorithms.

Given all other requirements are fulfilled, I propose to award the candidate the title "Doctor of Philosophy".

Additional questions for a discussion:

1. On page 10, in step 13 of the CMA-ES algorithm, the covariance matrix is updated such that

the covariance matrix of unsuccessful mutations C_{μ}^{-} is subtracted in the last step. Cannot this subtraction, theoretically, cause the covariance matrix to loose its positive definitness? Does it happen in practice? How often? What happens in the algorithm if this happens?

- 2. Personally, I do not like the usage of the normalized Δ_f^{\log} score throughout the thesis because of the following reasons:
 - (a) The normalization makes the results relative to all the algorithms whose results are used. If the composition of the compared algorithms changes, the results of the same algorithm may be different.
 - (b) The normalization may incorrectly emphasize the differences among the results of the algorithms although the differences may be in fact quite negligible.
 - (c) It may also make a false impression that value 10^{-8} (used in BBOB and COCO framework as the final target) was achieved.

Could you react to these objections?

3. Could the classification trees in Figs. 40 and 41 be used to construct an algorithm with adaptive switching of surrogate models? If yes, why you did not make such a final evaluation and comparison to other algorithms? If no, what ingredients are still missing to perform such tests?

In Prague, September 26, 2022

Petr Pošík, Ph.D., examiner