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Evaluation by Michael T. M. Emmerich of HABILITATION THESIS
Martin Pilát
"Evolutionary Algorithms for Expensive
Optimization"
Department of Theoretical Computer Science and Mathematical Logic
Prague

Direct number 0031626501797

Date 18.5.2023

First, let me state that I enjoyed reading this interesting thesis in my research field, which is surrogate-assisted single- and multi-objective optimization.

Regarding the general comments on the thesis of Dr. Pilát:

Writing style and quality: The thesis is well-written and clearly indicates chapters based on publications. By publishing in top-ranked (peer-reviewed on the full paper) computer science conferences and journals (including ACM-GECCO, IJCNN, PPSN), the author has demonstrated the competitive international level of their scientific work.

Scientific Originality: The turnitin report indicates no significant indications of lack of originality in Dr. Pilát's work. The author clearly cites their published work in the thesis. The results are reported in a reproducible manner, and the ideas extend the state-of-the-art. Thus, the scientific integrity and originality of the work are established.

This thesis is divided into two parts, providing a comprehensive exploration of evolutionary algorithms and their applications. The first part covers essential background information through three informative chapters. Chapter 2 introduces evolutionary algorithms and addresses challenges associated with optimizing slow or expensive objective functions. Chapter 3 explores the implementation of evolutionary algorithms in parallel, especially when dealing with variable evaluation times. Chapter 4 focuses on surrogate models and their role in accelerating evolutionary algorithms, particularly in continuous optimization and genetic programming.

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The second part of the thesis comprises selected papers grouped into four chapters based on their respective topics. Chapter 5 serves as a bridge between the two parts, summarizing the main results of the papers and providing context within the broader research landscape. The papers cover various aspects of evolutionary algorithms, including parallelization, surrogate models in genetic programming, user preference consideration in multi-objective optimization, and solving problems with complex objective functions.

The major results of the author include:

1) Parallelization: The author presented an evolutionary algorithm with interleaving generations to improve parallelization, addressing the evaluation time bias in asynchronous algorithms. They also discussed the use of heterogeneous island models as parallel portfolios with automated algorithm selection. It is innovative research, and important as asynchronous strategies have the advantage to make full use of compute power. It has however be long researched in the past, and there is a danger of re-inventing the wheel (Island Models by Joachim Sprave (Ph.D. Thesis, TU Dortmund), Asynchronous Evolution Strategies with Median Selection (Wakunda et. al). Although I welcome more research in this important direction, it is necessary to refer to the established results in early works of evolutionary strategies to avoid repetition.
   Wakunda, Jürgen, and Andreas Zell. "Median-selection for parallel steady-state evolution strategies." *Parallel Problem Solving from Nature PPSN VI: 6th International Conference Paris, France, September 18–20, 2000 Proceedings 6*. Springer Berlin Heidelberg, 2000.
2) Surrogate Modelling: The author discussed two techniques for implementing surrogate models in genetic programming. One technique involved statically extracting features from genetic programs, while the other utilized modern graph neural networks. These techniques enable quality prediction without evaluating the program itself, proving valuable in complex evaluation scenarios such as automated machine learning.
   I consider this work as breaking new grounds in the topic of surrogate assisted optimization. The surrogate models that are used in the literature require mainly parametric inputs, and some work on combinatorial and mixed integer spaces. But the application to grammatically defined representations seem to be novel. In drug discovery there are some examples (molecules, not programs) that also feature grammatical search spaces and utilize graph-neural networks for prediction, but to my knowledge these predictions are not used in optimization.
3) User Preference Consideration: The author presented a multi-objective evolutionary algorithm that incorporates co-evolution to consider user preferences. This enhances the algorithm's effectiveness by avoiding unnecessary computation on uninteresting individuals.
   I am a bit uncertain about judging the impact of this result, but it is surely original approach to use co-evolution, and it is in row with a series of papers by various authors on interactive and preference based MOEAs.
4) Applications in Complex Objective Functions: The author demonstrated the application of evolutionary algorithms in various problem domains, including

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automated machine learning, coordinated charging of electric vehicles, and finding adversarial examples in image classification with deep neural networks, adversarial counterexamples.
I think that this part of the thesis demonstrate, how versatile the approach is and that it can be adopted to various topics of recent technological research (electro-mobility, deep learning architectures). In applications the challenge is to make things work and produce competitive results in the application domain. The applications that the author has included in the thesis are clearly non-trivial and showcase the power of the advanced evolutionary algorithm frameworks.

Regarding future work, the author intends to: Focus on problems with expensive objective functions, particularly in rapidly developing areas like automated machine learning and neural architecture search.

1. Continue research on surrogate models, exploring their application beyond continuous optimization, especially in genetic programming.
2. Expand parallel implementations of evolutionary algorithms, particularly in multi-objective optimization scenarios where objectives may have varying evaluation times.
3. Further investigate applications of evolutionary algorithms in areas such as machine learning, automated machine learning, neural architecture search, and adversarial examples.

It is worth noting that the author's future research directions show promise, but there are already existing works in some areas, such as the Ph.D. thesis of Richard Allmendinger (Manchester University on heterogeneous objectives) and distinguishing the new work from the existing literature will be important. Additionally, the application of evolutionary algorithms in engineering design optimization, computational medicine, and real-world dynamic combinatorial optimization is crucial and presents significant challenges, next to the ones mentioned by the author.
In addition, the field of artificial intelligence, including evolutionary computation, would greatly benefit from techniques that promote mathematical rigor and reproducibility. Incorporating well-motivated benchmarks and statistical hypothesis tests would facilitate the building upon previous research by authors. Currently, there is a lack of exact results and carefully tested hypotheses within the field, and future work should address this issue. While Dr. Pilát's work sets a positive example of reporting results, (research in) establishing standards for registering new findings is still necessary to enable other scientists to build upon earlier research. Perhaps, digital tools can also help to automatize this registration of results.

In summary, the habilitation thesis of Dr. Pilát is convincing me, and I suggest that it can be accepted without the need of modifications.

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