

Designing new metaheuristic implementations: from metaphors to automatic design

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A metaheuristic is a general algorithmic framework that can be easily adapted to many different optimization problems for which exact/analytical approaches are either limited or impractical. There are two main approaches used to create new metaheuristic implementations: *manual design*, which is based on the designer's "intuition"—often involving looking for inspiration in other fields of knowledge—and *automatic design*, which seeks to remove human intervention from the design process by harnessing recent advances in automatic algorithm configuration methods and machine learning. Compared to manual design, which is typically time-consuming and error-prone, automatic design is often much more efficient and has advantages, such as removing biases from the creation process and increasing the flexibility with which new metaheuristic designs can be explored. Yet, to this day, the vast majority of metaheuristics proposed in the literature are still created by algorithm designers who manually define the different components that make up the implementation based on their knowledge (empirical, theoretical or intuitive) and/or by considering new sources of inspiration.

The main topic of the thesis is how to improve the way we create metaheuristics by replacing manual design with automatic design. We focus especially on those cases where the use of manual design involves taking inspiration from natural and even supernatural behaviors, since this approach has been used intensively in the last two decades, spawning hundreds of so-called "novel" metaphor-based metaheuristics. Unfortunately, for the vast majority of them, it is still unknown what is their real novelty apart from the use of the new metaphors. In order to put an end to this situation and, indeed, to try to remedy it, we advocate for replacing "intuition" and "new sources of inspiration" with automated design methods. To demonstrate the feasibility of this approach and its advantages, we develop a metaheuristic software framework with a modular design, that is coupled with an automatic configuration tool and allows to automatically create high-performing implementations with novel designs.

In the first half of the doctoral thesis, we focus on studying how the process of designing metaheuristics has changed over the years. In doing so, we identify the limitations of the approach of looking for inspiration in other fields of knowledge and establish clear criteria to determine the cases where considering introducing new metaphors makes *sense* and those where it does not. In this endeavor, we rigorously analyze some of the most widespread and highly-cited “novel” metaphor-based metaheuristics proposed in the last years, and compare their components with those defined in some of the best-known metaheuristics that have been proposed in the literature. We show that, despite being presented as *novel* optimization techniques, they are in fact the same as, or at best minor variations of, classic approaches, many of which were proposed years, or even decades, before the “novel” metaheuristics were published.

In the second half of the thesis, we explore the use of automatic design as a powerful alternative to manual design, that has also the potential of rendering the need to find new sources of inspiration obsolete. We describe how modular metaheuristic software frameworks are created, what are their advantages and challenges, and why they are the most efficient way we have at the moment to try to come up with new metaheuristic designs. We experimentally demonstrate that the metaheuristic software framework for particle swarm optimization that we developed in the context of this research work can be used to create high-performing implementations whose design had never been considered before in the literature, without the need for introducing new sources of inspiration, or any other kind of manual intervention. This doctoral thesis concludes by: (i) identifying ways in which some of the fundamental aspect of the broad field of metaheuristics can be improved; (ii) discussing the research contributions presented in this work; and (iii) identifying some research paths that can be explored in the future to extend the results presented in this doctoral thesis.

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Declarations

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