pysamoo: Surrogate-Assisted Multi-Objective Optimization in Python

Julian Blank and Kalyanmoy Deb

Abstract—Significant effort has been made to solve computationally expensive optimization problems in the past two decades, and various optimization methods incorporating surrogates into optimization have been proposed. However, most optimization toolboxes do not consist of ready-to-run algorithms for computationally expensive problems, especially in combination with other key requirements, such as handling multiple conflicting objectives or constraints. Thus, the lack of appropriate software packages has become a bottleneck for solving real-world applications. The proposed framework, pysamoo, addresses these shortcomings of existing optimization frameworks and provides multiple optimization methods for handling problems involving time-consuming evaluation functions. The framework extends the functionalities of pymoo, a popular and comprehensive toolbox for multi-objective optimization, and incorporates surrogates to support expensive function evaluations. The framework is available under the GNU Affero General Public License (AGPL) and is primarily designed for research purposes. For more information about pysamoo, readers are encouraged to visit: anyoptimization.com/projects/pysamoo.

Index Terms—Surrogate-Assisted Optimization, Model-based Optimization, Simulation Optimization, Evolutionary Computing, Genetic Algorithms.

I. EXPENSIVE OPTIMIZATION

Many optimization problems are computationally expensive and require the execution of one or multiple time-consuming functions to evaluate a solution. Expensive Optimization Problems (EOPs) are especially important in practice and are omnipresent in all kinds of research and application areas, for instance Agriculture [1], Engineering [2], Health Care [3], or Computer Science [4]. Often the expensiveness of the evaluation is caused by the requirement of running a simulation, such as Computational Fluid Dynamic (CFD) [5], Finite Element Analysis (FEA) [6], or processing a large amount of data [7], [8]. It is worth noting that the majority of simulation-based data-intensive problems are black-box in nature [9] and gradient information is not available or is even more time-consuming to derive. This makes it even more vital to address the time-consuming objective and/or constraint functions as an inherent part of the optimization problem and significantly limits the overall evaluation budget.

The execution of a time-consuming evaluation dominates the algorithm’s computational overhead for finding new solutions in each iteration. Thus, an algorithm has more time for carefully selecting new designs than traditional optimization algorithms; however, the evaluation budget is usually only limited to a few hundred evaluations instead of a few thousand evaluations. A standard method to speed up the convergence of existing methods is using a surrogate model (also called metamodel, approximation model, simulation model, data-driven model, response surface), which approximates the time-consuming function. Incorporating a surrogate into the optimization process is indicated by adding “surrogate-assisted” or “metamodel-based” to the algorithm’s name or description. The incorporation of surrogates into optimization is illustrated in Figure 1. Commonly, surrogates – approximation or interpolation models – are utilized during optimization to improve the convergence behavior. First, one shall distinguish between two different types of evaluations: Expensive solution evaluations (ESEs), which require running the computationally expensive evaluation, and approximate solution evaluations (ASEs), which is a computationally inexpensive approximation by the surrogate. Where the overall optimization run is limited by ESE\(_{\text{max}}\) function evaluation, function calls of ASEs are only considered as algorithmic overhead. The goal of surrogate-assisted optimization is to provide efficient ASEs with the least approximation error possible and to exploit them to minimize ESEs function calls. Thus, the overall goal is to improve the convergence of an optimization algorithm as much as possible in the usually very limited evaluation budget ESE\(_{\text{max}}\).

II. THE FRAMEWORK

Most researchers rely on open-source packages to conduct their research. Finding an appropriate open-source package can be quite challenging, especially when attempting to solve real-world and application problems. For optimization, one has to note that most optimization toolboxes do not consist of ready-to-run algorithms for computationally expensive problems. Moreover, other vital requirements, such as handling multiple conflicting objectives or constraints, are often not supported. The proposed framework, pysamoo, addresses these shortcomings of existing optimization frameworks and provides different types of optimization methods targeting time-consuming functions. The framework extends the functionalities of pymoo [10], a popular and comprehensive toolbox.
for multi-objective optimization, and incorporates surrogate support.

The framework includes implementations of PSAF [11] and GPSAF [12], which are two surrogate incorporation strategies (proposed by the authors of this paper) to generalize model assistance for all different types of metaheuristics. In the current version of the framework surrogates are incorporated into GA [13], DE [14], CMAES [15], ISRES [16] and NSGA-II [17], and NSGA-III [18], [19], [20] and others. The framework is available under the GNU Affero General Public License (AGPL) and is primarily designed for research purposes. For further information on the constituent PSAF and GPSAF algorithms which are in the core of pysamoo, refer to references [11] and [12], respectively.

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