Proposal for the Doctoral Program of the Sorbonne Center for Artificial Intelligence (SCAI)

Fighting High Dimensionality in Bayesian Optimization for Applications in Mechanical Design

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Abstract

Recent advances in innovative manufacturing technologies and computer-aided tools have focused attention on the prototyping phase of mechanical structures, where artificial intelligence can help automate workflows and limit human intervention. Since mechanical designs are usually characterized by very expensive numerical simulations, surrogate-based optimization techniques play a crucial role in their optimization. Unfortunately, the number of parameters that define a component under study can be very large. This poses a challenge for surrogate-based optimization, as the number of training samples that are needed to build reliable models increases exponentially with the dimensionality of the problem. Appropriate techniques to handle this *curse of dimensionality* are therefore at high demand.

In this PhD project, we aim at investigating new dimensionality reduction methods to improve the performance of Bayesian optimization for high-dimensional mechanical applications. Of particular interest are unsupervised learning techniques from the field of geometric deep learning, e.g., autoencoders, as well as the construction of low-dimensional manifolds via linear and nonlinear mappings.

1 Context

Mechanical engineering and artificial intelligence (AI) go hand in hand, as the systems that have emerged and will be created in the 21st century are a blend of the two. In particular, machine learning (ML) can be used to accelerate and improve material and geometry design processes. Because component development is now heavily supported by computational and software tools such as computer-aided design (CAD) and finite-element analysis (FEA), advances in AI can easily lead to higher levels of product automation and accelerated innovation of new products. Recently, there has been increased interest in black-box optimization (BBO) strategies for automating machine learning workflows with minimal human intervention. The ML model can be viewed as a black-box function, whose goal is to optimize performance criteria [1]. Moreover, complex black-box functions can themselves be interpreted as ML pipelines consisting of several steps, including pre-processing, dimensionality reduction, model selection and training, cross-validation, and post-processing [2]. In this context, several methods developed in recent years are based on surrogate models [3], which allow the construction of a computationally cheap-to-evaluate approximation of the considered expensive objective function under consideration, replacing the direct optimization of the real objective by the model. This is particularly useful in computational mechanics problems where each objective function evaluation requires a high-fidelity FEA simulation that may even take several hours to days, limiting the total budget of function evaluations that can be performed.

2 Project Description

Scientific Objective: Bayesian Optimization (BO) is a powerful sequential design strategy for global optimization of black-box functions, which is particularly suitable to address objective functions that are computationally expensive to evaluate. Built upon a so-called infill-criterion and Gaussian Process regression (GPR), BO suffers from a substantial computational complexity and hampered convergence rate as the dimension of the search spaces increases. Scaling up BO for high-dimensional optimization problems remains a challenging task. **The aim of this project is hence to develop efficient optimization algorithms using Bayesian optimization (BO) to address high-dimensional real-world applications in the field of computational mechanics.** As a secondary objective, we aim at exploring how well classical benchmark problems from the academic world (e.g., those provided in [4, 5]) reflect the complexity of mechanical design problems and if (or how) transfer learning from such test beds is possible.

Motivation: Due to the complexity of crash phenomena and the computational cost of numerical simulations, surrogate-assisted optimization – BO in our particular case – and dimensionality/complexity reduction techniques will be addressed. There are already some researches looking at this direction, however they all show some limitations. For instance, Bergstra et al. [6] introduced a non-standard BO method based on a tree of one-dimensional density estimators. Another study by Hutter et al. [7] used random forests models in BO to optimize up to 76 mixed discrete/continuous parameters for solving hard combinatorial problems. However, both these methods rely on weak uncertainty estimates, which can fail even for the optimization of very simple functions and lack theoretical guarantees. In the linear bandits case, Carpentier and Munos [8] proposed a compressed sensing strategy to attack problems with a high degree of sparsity. Also recently, Chen et al. [9] made significant progress by introducing a two stage strategy for optimization and variable selection of high-dimensional GPs. This, however, requires the relevant dimensions to be axis-aligned with an ARD kernel. Wang et al. [10] used random embeddings in BO to reduce the dimensionality of the problems without knowing a priori which are the important dimensions. However, they demonstrated that their method is able to optimize functions of extremely high extrinsic dimensionality, but only provided that they have low intrinsic dimensionality, which cannot be guaranteed when dealing with crashworthiness optimization. The same limitation is found in a recent study by Eriksson and Jankowiak [11], in which they present the Sparse Axis-Aligned Subspace BO (SAASBO) algorithm. SAASBO performs excellently on several synthetic and real-world problems, but its potential is only truly realized when the objective function depends strongly on just a subset of the variables that define the problem.

2.1 Project Organization

The sub-targets of this research are summarized in the following work packages:

- **WP1:** Implementation of complexity/dimensionality-reduction methods in the context of surrogate-based optimization. State-of-the-art machine learning methods will be investigated and integrated in the BO framework: good candidates are autoencoder neural networks [12], belonging to the domain of unsupervised machine learning, and principal component analysis, which demonstrated to be a valuable tool for reducing the dimensionality of a problem when coupled with BO and tested on multi-modal functions with an adequate global structure [13];
- **WP2:** Extensive testing on academic benchmark problems and empirical comparison with high-dimensional BO algorithms already available in the literature.
- **WP3:** Transfer learning from the extensive testing on artificial benchmarks to the optimization of real vehicle components (e.g., car hood, chassis, energy absorber) and crash structures in general. Knowledge from the previous mechanical and numerical tests will be embedded at this stage of the methodology;
- **WP4:** Enrichment of benchmark suites with problems that are representative of real-world problems in the field of mechanics.

2.2 Supervision

This project continues an ongoing collaboration between the LIP6 Department of Sorbonne University and the TUM Chair of Computational Mechanics, established in 2021 by means of a DAAD PRIME postdoctoral fellowship and a jointly supervised Master's thesis project. The PhD student will therefore integrate into an existing collaborative environment. The synergy between the two departments and the expertise of the supervisors fits perfectly with the interdisciplinary nature of the project, including optimization techniques and numerical modeling for mechanics, respectively.

Main Supervisor is **Carola Doerr**, formerly Winzen. Carola is since 2013 a CNRS researcher (HDR 2020) within the Operations Research team at LIP6, Sorbonne Université in Paris, France. Before joining the CNRS, she was a PostDoc at IRIF, Université de Paris, and at the Max Planck Institute for Informatics in Saarbrücken, Germany, where she obtained her PhD (Dr.-Ing.) *summa cum laude* in 2011 under the supervision of Kurt Mehlhorn.

Carola's main research activities are in the analysis of black-box optimization algorithms, with a strong focus on evolutionary algorithms and other sampling-based optimization heuristics.

Publications relevant to this proposal include [13] (BO using PCA dimensionality reduction), [14] (algorithm selection wizard built on top of Nevergrad), [15, 16] (IOHprofiler benchmarking platform providing detailed performance statistics and visualization) and [17] (award-winning entry in the 2020 NeurIPS black-box optimization competition, based on BO).

Co-Supervisor is **Fabian Duddeck**, associate professor at the Technical University of Munich (TUM). Fabian studied civil engineering at TUM, earning his Diplom (1990) and Dr.-Ing. in Mechanics (1997) there. After a postdoc period at École Polytechnique and at TUM, he acquired his habilitation in 2001. He later held an R&D position in industry (BMW) and served as lecturer at TUM. In 2005/6, he served as Reader (Associate

Professor) at Queen Mary University of London (QMUL) and as Maître de Conférences at École des Ponts ParisTech (ENPC). In 2010, he was appointed Professor for Computational Mechanics at TUM.

Fabian conducts research on the development of numerical methods for the simulation and optimization of structures, focusing on methods for parameter, shape, topology, layout, and material optimization of nonlinear and dynamic problems (acoustics, crash). New approaches for material modeling (composites, biomaterials) and the evaluation of aleatory and epistemic uncertainties (flexibility, robustness, reliability) complement these activities, often in the context of multi-physics and multi-disciplinary applications.

Publications relevant to this proposal include [18, 19] (Surrogate-based topology optimization of mechanical structure in statics and crashworthiness), [20] (Methods to reduce design complexity), and [21] (Deep autoencoder networks for the identification of topological prototypes).

2.3 Sought Student Profile

The candidate should have a Master's degree in a quantitative field (e.g., Computer Science, Engineering, Mathematics, Statistics, Operations Research or other related field), experience with at least one programming language (e.g., Python, R, Java, or C++), and should be willing to conduct empirical work in the intersection of optimization and computational mechanics. Previous experience with finite element pre/post-processing software, CAD, and solver interfaces would be an asset. Since the student will be working in an international research team, they must be proficient in written and spoken English. Knowledge of French is not required. International students are very welcome to apply.

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