Cenaero

Ref.: BE-IP-2025-002

Internship Proposal

Improvement of kernel-based models by means of selection and aggregation strategies in surrogate-based optimization

Cenaero, located in Gosselies (Belgium), is a private non-profit applied research center providing companies involved in a technology innovation process with numerical simulation methods and tools to invent and design more competitive products. Internationally recognized, in particular through its research partnership with Safran, Cenaero is mainly active in the aerospace (with an emphasis on turbomachinery), process engineering, energy and building sectors.

Cenaero provides expertise and engineering services in multidisciplinary simulation, design and optimization in the fields of mechanics (fluid, structure, thermal and acoustics), manufacturing of metallic and composite structures as well as in analysis of in-service behavior of complex systems and life prediction. Cenaero also provides software through its massively parallel multi-physics platform Argo, its manufacturing process simulation and crack propagation platform Morfeo and its design space exploration and optimization platform Minamo.

Cenaero operates the Tier-1 Walloon supercomputing infrastructure Lucia with 4 Pflops peak performance and was ranked 245th on the November 2022 Top500 List (see tier1.cenaero.be for details).

Within Cenaero, the Machine Learning and Optimization group is dedicated to the development of algorithms and methods to address complex industrial design cases, with several achievements in aeronautics in particular [1-2]. It incorporates the Minamo team, dedicated to the development of Cenaero's in-house multi-disciplinary optimization platform. Although computing power has increased dramatically in the last decades, computational burden is still an issue as more and more complex simulation analyses are required in industrial design processes. Aiming to tackle this numerical challenge, Minamo provides efficient online Surrogate-Based Optimization (SBO) methods, based on evolutionary algorithms, allowing to quickly gain insight into the design space, to quantitatively identify key factors and trends and to automatically find innovative design options. It implements several variants of mono- and multi-objective evolutionary strategies, efficiently coupled in an online framework (i.e with continuous enrichment of the construction support along the design iterates) to surrogate models.

One of the key factors responsible for the success of a SBO approach is the choice / training process of the approximate model. The idea is to extract knowledge from the surrogates to find promising zones to satisfy constraints and minimize the objectives. The selection of the surrogate model, its optimization and enrichment are crucial for the approximate problem to fit the real design problem as closely and with as few intensive computations as possible.

Context

A classical SBO approach consists of several major components, as shown in Figure 1. The first step relates to the Design of Experiments (DoE) which provides data for the initial surrogate model training. The second step consists in the training of the surrogate model(s). The third aspect of such optimization techniques is the choice of the model updating strategy. The last step is the evaluation of the stopping criterion to determine whether a new iterate is needed or not. The aim of the surrogate is to allow for intensive evaluation of the approximate functions of interest [3]. Evolutionary Algorithms being known to be very intensive in terms of function evaluations for a global exploration of the design space, the surrogate models reduce the computational budget of the optimization scheme. The keys characteristics of a surrogate model include its training cost (in terms of number of training points and hyper-parameters optimization complexity), its predictability throughout the whole design space, and its capability to give an estimate of its own reliability in the design space. A wide variety of techniques are available to construct these surrogate models, such as Kriging or Radial Basis Function Networks (RBFN). Since several surrogate types can be available, *a priori* choosing the most suitable one for a given quantity of interest is a difficult task for the user. Therefore, the aim of this work is to investigate some automatic strategies that can help to select the "best" surrogate model, or to aggregate several surrogate models by weighting them with a "quality" factor, see [4]. These strategies of selection and aggregation of models allow to overcome the bias introduced by poorly choosen surrogate models. Indeed, one unique choice of surrogate model can not be suited to all kind of problems. Moreover, the same choice for all responses (objective(s) and constraint(s)) can be inadequate since the different responses can have very different behaviors and therefore require different types of approximation.

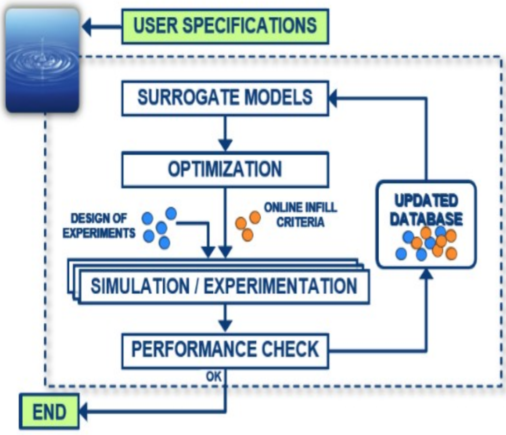

Figure 1: Online SBO scheme

Objective

The aim of this work is to:

- Perform a bibliographical review on selection and aggregation strategies (for instance [5, 6, 7]);
- Compare the existing surrogate models predictability on a set of carefully chosen test cases by means of different kernels choice in selection strategy;
- Implement new surrogate models selection/aggregations strategies;
- Compare the predictability and training costs of the developed surrogate models strategies on different mathematical problems.

Depending on the progress and results obtained during this internship, these strategies may be tested on a realistic benchmark related to wing design.

The candidate will join the Machine Learning & Optimization group.

Profile

- Required: Master's student in Mathematics, Engineering or Computer Science.
- Languages: English and/or French.
- Prerequisites: Good programming skills as well as good mathematical background. Working knowledge of Linux and Python are valuable assets.
- Motivation, creativity and team spirit!

Duration

The length of the internship can vary from 3 months to 6 months, depending on your university or school regulations.

Contact

If you are interested by this topic, please send a cover letter, quoting the reference number of the offer, as well as your resume, to rh_be-ip-2025-002@cenaero.be.

References

[1] Baert, L., Chérière, E., Sainvitu, C., Lepot, I., Nouvellon, A., Leonardon, V. *Aerodynamic Optimisation of the Low Pressure Turbine Module: Exploiting Surrogate Models in a High-Dimensional Design Space*. Journal of Turbomachinery. 142:1-24 (2020).

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[5] A. Díaz-Manríquez, G. Toscano-Pulido and W. Gómez-Flores, *On the selection of surrogate models in evolutionary optimization algorithms*, 2011 IEEE Congress of Evolutionary Computation (CEC), New Orleans, LA, USA, , pp. 2155-2162, (2011).

[6] Bianca Williams, Selen Cremaschi, *Selection of surrogate modeling techniques for surface approximation and surrogate-based optimization*, Chemical Engineering Research and Design, Volume 170, Pages 76-89, (2021).

[7] Müller, J., Shoemaker, C.A. *Influence of ensemble surrogate models and sampling strategy on the solution quality of algorithms for computationally expensive black-box global optimization problems*. *J Glob Optim* **60**, 123–144 (2014).