Processus Gaussiens pour l'analyse et l'optimisation des systèmes complexes

Soutenance de thèse – Ali Hebbal

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Salle Marcel Pierre - ONERA Palaiseau,
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Abstract :

In engineering, the design of complex systems, such as aerospace launch vehicles, involves the analysis and optimization of problems presenting diverse challenges. Actually, the designer has to take into account different aspects in the design of complex systems, such as the presence of black-box computationally expensive functions, the complex behavior of the optimized performance (abrupt change of a physical property here referred as non-stationarity), the multiple objectives and constraints involved, the multi-source information handling in a multi-fidelity framework, and the epistemic and aleatory uncertainties affecting the physical models. A wide range of machine learning methods are used to address these various challenges. Among these approaches, Gaussian Processes (GPs), benefiting from their Bayesian and non-parametric formulation, are popular in the literature and diverse state-of-the-art algorithms for the design of complex systems are based on these models.

Despite being widely used for the analysis and optimization of complex systems, GPs, still present some limitations. For the optimization of computationally expensive functions, GPs are used within the Bayesian optimization framework as regression models. However, for the optimization of non-stationary problems, they are not suitable due to the use of a prior stationary covariance function. Furthermore, in Bayesian optimization of multiple objectives, a GP is used for each involved objective independently, which prevents the exhibition of a potential correlation between the objectives. Another limitation occurs in multi-fidelity analysis where GP-based models are used to improve high-fidelity models using low-fidelity information. However, these models usually assume that the different fidelity input spaces are identically defined, which is not the case in some design problems.

In this thesis, approaches are developed to overcome the limits of GPs in the analysis and optimization of complex systems. These approaches are based on Deep Gaussian Processes (DGPs), the hierarchical generalization of Gaussian processes.

To handle non-stationarity in Bayesian optimization, a framework is developed that couples Bayesian optimization with DGPs. The inner layers allow a non-parametric Bayesian mapping of the input space to better represent non-stationary functions. For multi-objective Bayesian optimization, a multi-objective DGP model is developed. Each layer of this model corresponds to an objective and the different layers are connected with undirected edges to encode the potential correlation between objectives. Moreover, a computational approach for the expected hyper-volume improvement is proposed to take into account this correlation at the infill criterion level as well. Finally, to address multi-fidelity analysis for different input space definitions, a two-level DGP model is developed. This model allows a joint optimization of the multi-fidelity model and the input space mapping between fidelities.

The different approaches developed are assessed on analytical problems as well as on representative aerospace vehicle design problems with respect to state-of-the-art approaches.

Mots clés Gaussian Processes, deep Gaussian processes, Bayesian optimization, multi-objective optimization, multi-fidelity analysis, complex system design.