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Bayesian optimization for efficient parameter space coverage with computationally demanding simulations in fusion energy applications

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Magnetic confinement fusion research is characterized by computationally demanding physics models with a selection of uncertain, phenomenological input parameters. Rigorous usage of such models for predictive or interpretative applications requires a thorough inverse uncertainty quantification (UQ) for these input parameters [1]. Bayesian inference (BI) algorithms provide a principled approach to quantify the uncertainty, as a probability distribution, for the state of the investigated system or hypothesis validity, given the available information [2]. When operating with computationally costly models, data-efficiency is key to maximizing the information gain in establishing this probability distribution. Such efficiency can be achieved by combining "Bayesian optimization"(BO) with the overall BI task. BO is a powerful framework for data-efficient global optimization of costly, non-convex functions, without access to first- or second-order derivatives [3]. On the one hand, BO uses BI to build a statistical approximation in the space of functions that represents the costly model, leveraging the Bayesian quantification of uncertainty over functions to efficiently refine the approximation where needed. On the other hand, the overall BI task is focused on establishing posterior probability distributions over the uncertain state of the investigated system or hypothesis. Crucially, the overall BI task can be conducted with or without BO, but the application of BO renders the BI task orders of magnitude more data-efficient. For many practical applications in fusion energy research, batch BO is needed [4]. The standard BO algorithms conduct sequential search, where a computationally relatively light to evaluate acquisition function is optimized to recommend the highest utility sample to collect with the computationally demanding model. However, if evaluation of the full model takes longer than a few hours, which is quite typical in fusion research applications, the overall optimization time with a sequential approach can easily become unacceptably long. Batch BO can be used to collect several samples in parallel to each other, accelerating the overall optimization task to the throughput levels required for practical applications in fusion energy research. This work discusses BI and BO work performed within or in close connection to the EUROfusion Advanced Computing Hub, hosted by the University of Helsinki (ACH 5). The example applications presented in this work encompass runaway electron simulations [5, 6], scrape-off layer (SOL) plasma simulations, integrated plasma scenario simulations, and tokamak experiment design through BO algorithms [7].

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Speaker's Affiliation

VTT Technical Research Centre of Finland

Member State or IGO/NGO

Finland

Primary author: JÄRVINEN, Aaro (VTT)

Co-authors: Dr HO, Aaron (DIFFER); KIT, Adam (Helsinki University); Dr BHARTI, Ayush (Aalto University); Dr FURIA, Chirag (Brown University); Mr AMNELL, Emil (University of Helsinki); NARDON, Eric (CEA); Dr CLARTE, Gregoire (University of Helsinki); Prof. ACERBI, Luigi (University of Helsinki); HOPPE, Mathias (KTH); CHURCHILL, Randy (Princeton Plasma Physics Laboratory); Dr SILBURN, Scott (UKAEA); Prof. FÜLÖP, TÃ¼nde (Chalmers University of Technology)

Presenter: JÄRVINEN, Aaro (VTT)

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