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Subset selection of optimal solutions in settings with noisy outcomes, using Gaussian processes Co-author: Inneke Van Nieuwenhuyse

Bayesian optimization is an increasingly popular approach for optimizing expensive black-box problems in many fields (e.g., engineering, operations research, computer science). In Bayesian optimization, probabilistic metamodels (usually Gaussian Process models) are used to emulate the objective and/or constraint functions. These metamodels allow the analyst to predict the outcome of these functions throughout the search space, and can guide the search for the optimal solution in a data-efficient way (i.e., requiring as few as possible expensive observations).

Strikingly, the probabilistic nature of the metamodels is currently overlooked when identifying the best solution(s) at the end of the optimization: indeed, most Bayesian optimization approaches just return the solution with the best expected outcome. This presentation highlights the need for an identification approach that accounts for the uncertain nature of the metamodels, and proposes a subset selection approach (which returns all solutions in the search space that are estimated to be non-inferior) that is in line with the assumptions of Gaussian Process metamodels. We also illustrate the impact of an additional "accuracy phase", in which extra experiments are performed to improve the accuracy of the metamodels *before* moving on to the subset selection.

We illustrate the results of the subset selection approach (with and without accuracy phase) within the context of a simulation optimization problem. It can be used, however, in *any* setting where the analyst has a finite number of solutions for which uncertain outcomes are available (e.g., results of stochastic simulation experiments in operations management, or physical experiments in engineering), and to which Gaussian Process models can be fit. The current approach requires the search space to be discretized; future research will focus on how to relax this requirement.

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