Diverse Expected Improvement (DEI): Diverse Optimization of Expensive Black-box Simulators for Internal Combustion Engine Control

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The optimization of expensive black-box simulators arises in a myriad of modern scientific and engineering applications. Bayesian optimization provides an appealing solution, by leveraging a fitted surrogate model to sequentially guide simulator evaluations. In practical problems, however, the goal is often not to obtain a single good solution, but a "basket" of good solutions from which users can choose for downstream decision-making. This arises in our motivating application for real-time control of unmanned aerial vehicles (UAVs), where a diverse set of control strategies are desired for robust and timely control. Despite its importance, there has been little work on this front for Bayesian optimization. We thus propose a new Diverse Expected Improvement (DEI) method, which extends the well-known Expected Improvement method to encourage diversity between "ϵ-optimal" solutions, i.e., solutions with objectives within a small ϵ from a global optimum. The DEI jointly targets two goals: the exploration of ϵ-optimal regions on the solution space, and the exploitation of promising solutions that may improve upon the current best solution. One advantage of the DEI is that it admits a closed-form acquisition function under a Gaussian process surrogate model, which facilitates efficient sequential queries via automatic differentiation. We demonstrate the improvement of DEI over state-of-the-art methods for diverse optimization in a suite of numerical experiments. We then explore the DEI in two practical applications, the first on rover trajectory optimization and the second for real-time control of UAVs