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Possible Pitfalls in Using Bayesian Optimization (BO) to Quickly Optimize the Levels of Factors in a Physical Experiment

BO methods have recently been advocated as a newly accessible, straightforward, hands-off alternative to design of experiments (DOE) to efficiently optimize the levels of the factors in physical experiments. Physical experiments have random variation between replicated runs.

In the typical hands-on DOE approach to process optimization, an initial choice of factors and their ranges is made and an experimental design (classical or optimal) that enables an initial model to be fit is chosen. A significant model is fitted and used to optimize the process. Often a series of experiments are run, with the selection of factors and/or factor ranges adjusted. We assume (and check) that a simple linear or quadratic model plus random error will give a useful local approximation to the true relationship between the factors and the response/s.

The BO approach comes from the world of computer experiments, where both the nature of the problem and the solution strategy are very different. In this world, complex models are considered, random variation is non-existent or negligible, and runs are obtained one at a time or in small groups. An algorithm is used to efficiently explore a fixed design space with prescribed factors and ranges. Kriging models are automatically fitted and updated behind the scenes.

We consider possible pitfalls when using BO tools to optimize a real process with non-negligible random variation between runs. Can we start with only a handful of initial runs? Will variation cause the BO algorithm to fail? Will we know if it does fail?

Special/ Invited session

Classification

Both methodology and application

Keywords

DOE, BO, optimization

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