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Simulation-Optimization under Uncertainty through Metamodeling and Bootstrapping

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Abstract

Most methods in simulation-optimization assume known environments, whereas this research accounts for uncertain environments combining Taguchi's world view with either regression or Kriging (Gaussian Process) metamodels (response surfaces). These metamodels are combined with Non-Linear Mathematical Programming (NLMP) to find a robust optimal solution. Varying the constraint values in the NLMP model gives an estimated Pareto frontier. To account for the variability of the estimated Pareto frontier, this research uses bootstrapping which gives confidence regions for the robust optimal solution. This methodology is illustrated through the Economic Order Quantity (EOQ) inventory-management model, accounting for the uncertainties in the demand rate and the cost coefficients.

Keywords: Simulation-optimization; Uncertainty; Robustness; Metamodel; Bootstrap

1. Overview

Most methods in simulation-optimization assume known environments so all relevant parameters (simulation inputs) are known. Unfortunately, ignoring the uncertainty in some inputs of the simulation model may lead to a suboptimal solution. Robust optimization aims at deriving solutions that are relatively insensitive to perturbations in the model parameters.

In Taguchi's world view there are *decision factors*—which are under the control of management—and *environmental factors*—which are uncertain and are not controlled. Taguchi's work is meant for real-life experiments, whereas we consider simulation experiments: this gives us more flexibility, because we can explore many values per input and many scenarios (combinations of these values). Taguchi's statistical techniques have been seriously criticized; therefore, we do not use these techniques. To design our simulation study, we adopt a

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Design of Experiments (DOE) that combines (crosses) a Latin Hypercube Design for the environmental factors that accounts for their distribution function, and a space-filling design for the decision factors.

In our current research, we assume a single output of the simulation model. Because simulation runs are often computationally expensive, we approximate the Input/Output (I/O) function of the simulation model through a *metamodel*. Dellino *et al.* (2009b) integrate the Taguchian worldview and two metamodeling techniques, namely regression analysis and Kriging. Dellino *et al.* (2010) detail regression-based robust optimization, using the EOQ model for illustration. Inspired by Myers and Montgomery (1995), they fit a regression metamodel for the simulation output, accounting for interactions between decision and environmental factors. Next, they derive one regression metamodel for the expected mean of the simulation output and one regression metamodel for this output's standard deviation. The two metamodels are validated through leave-one-out cross-validation. Dellino *et al.* (2009a) replace regression analysis by Kriging; they compare two alternative Kriging approaches. In both approaches they fit one Kriging metamodel for the expected mean of the simulation output and one Kriging metamodel for its standard deviation.

To find robust optimal solutions, we formulate a *Non-Linear Mathematical Programming* (NLMP) problem as follows: our goal is to minimize the expected mean of the simulation output (through the corresponding metamodel), while keeping its standard deviation below a threshold. After solving this NLMP problem, we change the threshold within a given interval—properly chosen to reflect management's risk attitude—and solve the optimization problem for each value of the threshold. The set of resulting robust solutions estimates the Pareto frontier, trading-off the estimated mean and standard deviation of the simulation output.

The resulting Pareto frontier itself is uncertain: in fact, it has been estimated through simulation outputs corresponding to a sample of combinations for the environmental factors. To further analyze this frontier, we use *bootstrapping*. More specifically, we adopt parametric bootstrapping for our regression-based approach and distribution-free bootstrapping for our two Kriging-based approaches. In our regression approach we sample the regression parameters from a multivariate normal distribution with parameters estimated from the simulation data. In our Kriging approaches we resample—with replacement—the observed simulation output data, and recomputed the Kriging metamodels. To reduce the resulting sampling error, we repeat this sampling B times (e.g., $B = 100$). For further details on bootstrapping, we refer to Efron and Tibshirani (1993). Based on this bootstrapping, we obtain B fitted regression or Kriging metamodels for the expected mean and standard deviation of the simulation output. From these B observations we derive confidence intervals (see again Efron and Tibshirani 1993)., which quantify the variability of the metamodels. Next, we may compute confidence regions for each robust optimal solution belonging to the estimated Pareto frontier. Such a measure of variability can help management to choose a robust solution, not only accounting for its risk attitude but also for possible differences between estimated and actual values of the mean and standard deviation of the simulation output.

We test our new methodology through a popular inventory model, namely the EOQ model. We, however, introduce a robust formulation where the demand rate and the cost coefficients are uncertain. This example enables us to verify the performance of our heuristic because we can derive the *true* expected cost and its standard deviation. Furthermore, our results show the difference between our robust solution and the classic solution which ignores uncertainties in the environmental factors. Finally, the EOQ example gives encouraging results, which suggest the applicability of the methodology to more complex models.

2. References

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