Designing Computer Experiments to Determine Robust Control Variables

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Abstract

This manuscript is an extended abstract that outlines the problem solved in the paper of the same name that appears in *Statistica Sinica* and for which additional details are given in the technical report by Lehman et al. (2002).

Keywords: Computer experiments, Robust control variables, Expected improvement, Noise variables, Robust optimization, Sequential design

This research is concerned with the design of computer experiments when there are two types of inputs: control variables and environmental variables. Control variables, also called manufacturing variables, are determined by a product designer while environmental variables, called noise variables in the quality control literature, are uncontrolled in the field but take values that are characterized by a probability distribution. The *objective* is to design the computer experiment so as to find a set of *control variables* which are "robust" in the sense described below.

There are several different notions of robustness that have been proposed in the literature. To explain the current approach and its relationship to other approaches, suppose that $y(\cdot)$ denotes the output of the computer code and $\boldsymbol{x} = (\boldsymbol{x}_c, \boldsymbol{x}_e)$ denotes the input where $\boldsymbol{x}_c$ is the vector of control variables and $\boldsymbol{x}_e$ is the vector of environmental variables. Also let $F(\cdot)$ denote a tentative guess of distribution of the environmental variables, $\boldsymbol{X}_e$. If $F(\cdot)$ is known with *certainty*, we typically focus attention on determining either the distribution of $y(\boldsymbol{x}_c, \boldsymbol{X}_e)$ ("uncertainty analysis", see, for examples, O'Hagan and Haylock, 1997 or O'Hagan et al., 1999) *or* some summary of this distribution such as its mean $\mu(\boldsymbol{x}_c, F) = E_F\{y(\boldsymbol{x}_c, \boldsymbol{X}_e)\}$ (see, for example, Williams et al., 2000).

If $F(\cdot)$ is *unknown*, either completely or up to a finite vector of parameters, then $\mu(\boldsymbol{x}_c, F)$ may not be useful if its value is "sensitive" to the assumed $F(\cdot)$. The *minimax approach* to robustness assumes that a family $\mathcal{G}$ of distributions can be specified that contains the unknown $F(\cdot)$ (Huber, 1981). This approach defines $\boldsymbol{x}_c^{\mathcal{G}}$ to be $\mathcal{G}$*-robust* if

$$\max_{G \in \mathcal{G}} \quad \mu(\boldsymbol{x}_c^{\mathcal{G}}, G) = \min_{\boldsymbol{x}_c \in \mathcal{X}_c} \max_{G \in \mathcal{G}} \; \mu(\boldsymbol{x}_c, G).$$

Minimax robustness adopts a pessimistic viewpoint because it attempts to guard against the worst-case scenario among all $\boldsymbol{X}_e$ distributions in $\mathcal{G}$. The *Bayesian approach* to robustness focuses on the mean

$$\mu^{\Pi}(\boldsymbol{x}_c) = \int_{G \in \mathcal{G}} \mu(\boldsymbol{x}_c, G) \, d\,\Pi(G), \tag{1}$$

over the possible $\boldsymbol{X}_e$ distributions in $\mathcal{G}$; here $\Pi(\cdot)$ is a prior distribution on $\mathcal{G}$. A $\boldsymbol{x}_c^{\Pi}$ that minimizes (1) is said to be Π-*robust*.

Lehman et al. (2004) adopts a *Taguchi-like approach* to robustness. Assuming that interest lies in $\mu(\boldsymbol{x}_c, F)$, the idea of this type of robustness is that if $y(\boldsymbol{x}_c, \boldsymbol{x}_e)$ is relatively "flat" in $\boldsymbol{x}_e$ for a *given* $\boldsymbol{x}_c$ value, then the mean of $y(\boldsymbol{x}_c, \boldsymbol{X}_e)$ will be relatively independent of the choice of $F(\cdot)$ (and thus be robust to misspecification of $F(\cdot)$). Formally, we quantify the flatness of $y(\boldsymbol{x}_c, \boldsymbol{X}_e)$ by $\sigma^2_G(\boldsymbol{x}_c) = \text{Var}_G[y(\boldsymbol{x}_c, \boldsymbol{X}_e)]$, where $G(\cdot)$ is a user-selected distribution on $\boldsymbol{X}_e$. We define $\boldsymbol{x}_c^M$ to be M*-robust* if $\boldsymbol{x}_c^M$ minimizes $\mu(\boldsymbol{x}_c, F)$ subject to a constraint on $\sigma^2_G(\boldsymbol{x}_c)$. Alternatively, and perhaps more in keeping with the quality control concept of having a "target" mean, we define $\boldsymbol{x}_c^V$ to be V*-robust* if it minimizes $\sigma^2_G(\boldsymbol{x}_c)$ subject to a constraint on $\mu_F(\boldsymbol{x}_c)$.

Lehman et al. (2004) present sequential strategies for determing $\boldsymbol{x}_c^M$ and $\boldsymbol{x}_c^V$ based on a notion of "expected improvement" to select successive inputs to the computer code (Schonlau, 1997; Schonlau et al., 1998; Williams et al., 2000). The approach is Bayesian viewpoint. The computer code is treated as a realization of a Gaussian stochastic process; this random function model is the basis for interpolating the response based on a small training sample of computer runs (Sacks et al., 1989; Koehler and Owen, 1996). The predictive interpolator is used in place of the computer code to investigate the input–output relationship. The paper concludes by illustrating the performance of the algorithms proposed with examples that involve several different experimental goals. For the reader's convenience, the entire reference list for the published paper is given below.

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