Sequential Design of Computer Experiments Having Multiple Responses to Find a Constrained Optimum

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Abstract: This paper proposes a sequential method of designing computer experiments when the goal is to optimize one integrated response function subject to constraints on the integral of a second response function. This setting occurs naturally in industrial problems where the computed responses depend on two types of inputs: manufacturing variables and noise variables. If $\boldsymbol{x}$ is the vector of input variables then $\boldsymbol{x} = (\boldsymbol{x}_c, \boldsymbol{x}_e)$ where $\boldsymbol{x}_c$ is the set of manufacturing variables and $\boldsymbol{x}_e$ is the set of noise variables. In industrial settings, manufacturing variables are controlled by the product designer while noise variables are not controllable but have values governed by some probability distribution. If the bivariate response is $(z_1(\boldsymbol{x}), z_2(\boldsymbol{x}))$, then $\ell_i(\boldsymbol{x}_c) = \mathrm{E}[z_i(\boldsymbol{x}_c, \boldsymbol{X}_e)]$, the average response of $z_i(\boldsymbol{x}_c, \boldsymbol{X}_e)$ over the distribution of the environmental variables, is the integral of interest for $i = 1, 2$. We introduce a sequential design for selecting input values $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots$, at which to evaluate $(z_1(\boldsymbol{x}), z_2(\boldsymbol{x}))$ when the goal is to find the minimum of $\ell_1(\boldsymbol{x}_c)$ subject to $\ell_2(\boldsymbol{x}_c) \leq U$. Our approach is Bayesian; the prior specifies that the responses are a draw from a covariance stationary bivariate Gaussian stochastic process with correlation function belonging to a parametric family with unknown parameters. In addition, our models allow measurement error; thus the results can be applied to both computer and physical experiments. The proposed method selects the control portion of the next input site to maximize (over uncomputed input sites) a posterior expected "improvement" and the environmental portion of the next input to minimize the mean squared prediction error of the objective function at the new control site. The general formulas that are derived for the expected improvement and mean squared prediction error are specialized for an autoregressive-type prior model. The efficacy of the algorithm relative to single-stage design is illustrated in a deterministic setting; implementation issues for the deterministic and measurement error cases are discussed.