Williams, Brian J.; **Santner, Thomas J.**; **Notz, William I.**

Sequential design of computer experiments to minimize integrated response functions. (English) Zbl 0961.62069

Stat. Sin. 10, No. 4, 1133-1152 (2000).

Summary: In the last ten to fifteen years many phenomena that could only be studied using physical experiments can now be studied by computer experiments. Advances in the mathematical modeling of many physical processes, in algorithms for solving mathematical systems, and in computer speeds, have combined to make it possible to replace some physical experiments with computer experiments. In a computer experiment, a deterministic output, $y(x)$, is computed for each set of input variables x.

This paper is concerned with the commonly occuring situation in which there are two types of input variables: suppose $x = (x_c, x_e)$ where x_c is a set of "manufacturing" (control) variables and x_e is a set of "environmental" (noise) variables. Manufacturing variables can be controlled while environmental variables are not controllable but have values governed by some distribution. We introduce a sequential experimental design for finding the optimum of $\ell(x_c) = E\{y(x_c, X_e)\}$, where the expectation is taken over the distribution of the environmental variables. The approach is Bayesian; the prior information is that $y(x)$ is a draw from a stationary Gaussian stochastic process with correlation function from the Matérn class having unknown parameters.

The idea of the method is to compute the posterior expected "improvement" over the current optimum for each untested site; the design selects the next site to maximize the expected improvement. The procedure is illustrated with examples from the literature.

MSC:

62L05 Sequential statistical design
65C60 Computational problems in statistics (MSC2010)

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control variables; expected improvement; noise variables; optimization; computer experiments