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OPTIMAL DESIGN OF EXPERIMENTS WITH SIMULATION MODELS OF NEARLY SATURATED QUEUES

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Optimal design of experiments with simulation models of nearly saturated queues

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Abstract

The paper develops an approach to the optimal design of experiments with simulation models of nearly saturated queues, suggested in (Cheng, Kleijnen, 1996). This approach is based on the introduction of a regression model of the input-output behavior of the underlying simulation model. In this way the problem is reduced to a special regression experimental design problem. An analytical solution is found under some assumptions for the regression function and the behavior of the output variance. In particular D-optimality designs are considered and the solution is given for this case.

Key words: simulation, econometrics, queueing systems, metamodel, regression analysis, optimal experimental design

JEL: C0

ERN: econometrics, industrial organization and regulation

1. Introduction

The purpose of this paper is the development of a technique for simulating systems with nearly saturated queues. The naive simulation of such systems is impractical, since it will take a tremendous amount of computer time to accurately study such simulations.

At present, one of the main techniques for simulation studies of such systems consists of the simulation of an auxilary process. Such a process is either one which allows the estimation of corrections to theoretical models obtained by the diffusion approximation method (Minh, 1987), or one which corresponds to the importance sampling technique with a transformation function obtained by the solution of an integral equation (Asmussen, 1990). In both cases the approach assumes that an exact theoretical description of the model under investigation is possible, so it can be thoroughly analyzed by analytical techniques. This seems to be a very restrictive assumption.

One of the alternative approaches to the problem consists of the introduction of a regression model as a metamodel of the input-output behavior of the underlying complicated simulation model (Kleijnen, 1992; Cheng, Kleijnen, 1996). The main idea of this approach consists of the construction of a regression model for the forecast of a system behaviour with heavy traffic. Since the direct simulation is almost impossible, the system is simulated with a number of moderate traffic intensities and the results are used for the regression model building.

The theoretical ground for this approach is the fact that characteristics of queueing systems are quite smooth functions of the input variables and their behavior in a neighborhood of a critical point has a typical form that can be studied by analytical techniques. In a proceedings paper (Cheng, Kleijnen, 1996) a review of this matter was given. In that paper a class of regression models (to be described in the following section) was introduced, and a number of simulation experiments for academic examples of queues was performed to test if this class is appropriate. These simulation studies showed that the approach is practically realistic. In this approach the problem of system investigation is reduced to the estimation of regression model parameters. And the problem of the design of computer experiments is reduced to a special regression design problem. For its solution the paper introduced a number of numerical techniques. The present paper is devoted to the analytical solution of the same problem, under some restrictions for the regression model.

2. Statement of the problem

Let the behavior of a nearly saturated queueing system be studied by simulation. The usual M/M/1, M/G/1, and GI/G/m models can be considered as academic examples. The purpose of the study is the estimation of the expected queue length or the expected waiting time or, in more general terms, the estimation of the expected value of a linear functional. This expected value is estimated from the simulated sample paths.

Consider the approach based on the reduction of the problem to an optimal regression design problem. It is assumed that the simulation experiment is made up of a number of independent runs. It is further supposed that y, the output (response) of a run, is determined by x, a single independent input variable, and this input-output relationship can be represented by the following regression metamodel (response surface):

$$y_{ij} = g(x_i, \theta) + \epsilon_{ij}, \quad j = 1, \ldots, m_i, i = 1, \ldots, n \tag{1}$$

where ϵ denotes the approximation error of the metamodel, with mean $h(x_i)$ and variance $\sigma^2\varphi^2(x_i)$, $\theta = (\theta_0, \ldots, \theta_k)^\top$ is a vector of $k+1$ unknown parameters representing input effects, g, φ, h are known functions.

Let simulation runs be performed at n distinct input values $x_1, \ldots, x_n$ with m_i observations placed at the i-th point, $x_i (i = 1, \ldots, n)$. Denote the total number of runs by $N = \sum_1^n m_i$.

Consider the particular problem with $h(x) = 0$,

$$g(x, \theta) = (\theta_0 + \theta_1 x + \ldots + \theta_k x^k)/(1 - x), \tag{2}$$

$$\varphi(x) = 1/(1 - x)^2 \tag{3}$$

In (Cheng, Kleijnen, 1996) a general form for $Var(y/x)$ was considered. A case of particular interest is $Var(y/x) = const/(1 - x)^4$. This assumption is theoretically grounded in (Whitt, 1989) for the case of $M/M/1$ system where x is the input rate, the rate of service equals one, y is the mean length of queue and x is close to 1, and for more general cases by simulation experiments. We shall assume this particular form for $Var(y/x)$ in this paper. Note that the model for the variance will influence only the degree of optimality of estimators and designs.

Replacing y by $z = y(1 - x)^2$ gives

$$E(z/x) = (\theta_0 + \theta_1 x + \ldots + \theta_k x^k)(1 - x), \tag{4}$$

$$Var(z/x) \equiv \sigma^2, \tag{5}$$

where σ^2 is an unknown parameter. We can also assume that errors corresponding to distinct runs are independent random values. The vector of parameters θ can be estimated by the least squares technique. Denote this estimator by $\hat{\theta}$. Its optimality properties for models such as (4) - (5) are well known (see, for example, Rao, 1966).

Thus the problem is reduced to the optimal choice of $\{x_1, \ldots, x_n; m_1, \ldots, m_n\}$. It may be assumed that the optimality criterion is

$$Var(\hat{\theta}_0 + \hat{\theta}_1 + \ldots + \hat{\theta}_k), \tag{6}$$

which corresponds to the numerator in the right hand side of (2) with $x = 1$ since we are interested mainly in the behavior of the model for x close to 1.

Model (4) - (5) and criterion (6) were introduced in (Cheng, Kleijnen, 1996). In this paper it was shown that this model with $k = 2$ is appropriate for studying a systems of the type $M/M/1$ with the service discipline: first come first served. For other service disciplines it was proved that the model is appropriate with $k = 3$ or 4.

Let us study the problem for arbitrary (but fixed) k. For example, we may assume that k is chosen as a result of preliminary experiments.

Denote by ξ a discrete probability measure determined by the set $\{x_1, \ldots, x_n; \mu_1, \ldots, \mu_n\}$, where $\mu_i > 0, \sum \mu_i = 1, n$ is an arbitrary natural number, $x_i \neq x_j (i \neq j)$ are the points of segment $[0, 1]$. Without loss of generality we may assume that $0 \leq x_1 < x_2 <$

$\ldots < x_n \leq 1$. Such a measure is usually called an (approximate experimental) design since we can obtain integer numbers $\{m_i\}$ as rounded magnitudes $\mu_i N, i = 1, \ldots, n$. For simulation experiments, instead of rounding, we can chose the length of the runs to be proportional to μ_i for input values $x_i \quad (i = 1, 2, \ldots, n)$. In this case the term approximate loses its sense. The formal mathematical problem consists of finding a design $\xi^* = \{x_1^*, \ldots, x_n^*; \mu_1^*, \ldots, \mu_n^*\}$ such that the corresponding variance in (6) attains its minimal value, among all possible designs with $x_i \in [0, 1]$.

Besides criterion (6) we can use the D-optimality criterion. This consists of finding a design which maximizes the magnitude of the determinant of the information matrix. Statistical validity of the D-criterion is well known in regression design theory (see, for example, Karlin, Studden, 1966). Certainly, the D-optimal criterion is not specially adapted to the case of nearly saturated queues but can be considered in a general context of queues studying.

In the next section we shall obtain an analytical solution for both criteria.

3. Analytical solution of optimal designs

Let us introduce the following notations:

$$f(x) = (1, x, \ldots, x^k)^T, \text{ vector of basic functions,}$$
$$M(\xi) = \textstyle\sum_{i=1}^n f(x_i) f^T(x_i)(1 - x_i)^2 \mu_i, \text{ information matrix,}$$
$$T_{2(k+1)}(x) = cos((2k + 2) arccos x), \text{ Tchebysheff polynomial.}$$

Note that

$$Var(\hat{\theta}_0 + \hat{\theta}_1 + \ldots + \hat{\theta}_k) = Var f^T(1)\hat{\theta}. \tag{7}$$

The form of a design that minimizes (7) is given by the following theorem.

Theorem 1. *For regression model (4) — (5) a design ξ^* that minimizes (7) exists, is unique, and has the following form: $n = k + 1$,*

$$x_i^* = \frac{1}{r^2} cos^2(\pi(i-1)/(2k+2), r = cos(\pi/4k + 4),$$

$$\mu_i^* = \frac{|\, L_i(1) \,|}{1 - x_i^*} \Big/ \sum_{j=1}^{k+1} \frac{|\, L_j(1) \,|}{1 - x_i^*},\ i = 1, \ldots, k+1,$$

where $L_i(x)$ are Lagrange's interpolation polynomials, constructed from the points $\{x_i^*\}$:

$$L_i(x) = \prod_{j \neq i} (x - x_j^*) \Big/ \prod_{j \neq i} (x_i^* - x_j^*).$$

Additionally, for the optimal design

$$Var f^T(1)\hat{\theta} = \left(\sum_{j=1}^{k+1} \frac{|\, L_j(1) \,|}{1 - x_j^*} \right)^2 \sigma^2.$$

Note that the optimal design points are expressed through the extremal points of $T_{2k+2}(x)$; the proof of theorem 1 is similar to that of the theorem on extrapolation designs (see, for example, Karlin, Studden, 1966, Ch. X). Nevertheless since the proof need some additional arguments we give it in the Appendix.

Let us consider another criterion: design ξ^* is called D-optimal if

$$det M(\xi^*) = \max_{\xi} det M(\xi),$$

where maximum is spread over all designs with $x_i \in [0,1]$.

By the Kiefer-Wolfowitz equivalence theorem (see, for example, Kiefer, 1974) this design minimizes the magnitude

$$\max_{x} Var f^T(x)\hat{\theta}(1-x).$$

The form of D-optimal designs is given by the following theorem.

Theorem 2. *A D-optimal design ξ^* for model (4) — (5) exists, is unique, and has the following form:* $n = k+1$,

$$x_i^* = (y_i^*)^2, \mu_i^* = 1/(k+1), i = 1, 2, \ldots, k+1,$$

where $y_1^* = 0; y_2^*, \ldots, y_{k+1}^*$ are positive extremal points of Legendre's polynomial with parameter 1 *and degree* $2k+2$.

Proof. The existence of D-optimal designs is obvious. It is easy to check (similar to the corresponding assertion in (Karlin, Studden, 1966, ch. 10.6)) that any D-optimal design has $n = k+1$ points with equal weights. For such designs we have

$$\begin{aligned} det M(\xi) &= \frac{1}{(k+1)^{k+1}} det^2(x_i^{j-1}(1-x_i))_{i,j=1}^{k+1} \\ &= \frac{1}{(k+1)^{k+1}} \prod_{i=1}^{k+1}(1-x_i)^2 \prod_{i<j}(x_i - x_j)^2. \end{aligned}$$

The maximum of the last expression is achieved at the points given in theorem 2 (as it is proven in the Karlin, Studden, 1966).

4. An example: $k = 1$.

Let us illustrate Theorem 1 for the case $k = 1$. We have

$$r = cos\frac{\pi}{8} = \frac{\sqrt{2}}{4} + \frac{1}{2}, \quad x_1^* = 0, \quad x_2^* = cos^2\frac{\pi}{4}/r^2 = 2 - \sqrt{2},$$

$$L_1(1) = \frac{1 - x_2^*}{x_1^* - x_2^*} = \frac{\sqrt{2}-1}{\sqrt{2}-2}, \quad L_2(1) = \frac{1 - x_1^*}{x_2^* - x_1^*} = \frac{1}{2-\sqrt{2}},$$

$$\mu^* = \frac{|L_1(1)|}{1-x_1^*} \Big/ \left(\frac{|L_1(1)|}{1-x_1^*} + \frac{|L_2(1)|}{1-x_2^*}\right) = \frac{(\sqrt{2}-1)}{(\sqrt{2}-1)^2+1} = \frac{3-2\sqrt{2}}{4-2\sqrt{2}},$$

$$\mu_2^* = 1 - \mu_1^* = 1/(4-2\sqrt{2}).$$

By Theorem 2 for the case $k = 1$ we have

$$x_1^* = 0, x_2^* = 1/2, \mu_1^* = 1/2, \mu_2^* = 1/2.$$

It is worth pointing out that an experiment at the point $x_1^* = 0$ means that we simply investigate a system variant without any queueing if y is interpreted as the mean duration time of a job in the system or as the mean number of jobs in the system. If such an interpretation is not available, it proves necessary to modify the problem. The simplest way may be as follows. Let us take $\theta_0 = 0$ and replace the design $\{x_1^*, \dots, x_n^*; m_1^*, \dots, m_n^*\}$ by another one $\{x_1', \dots, x_{n'}'; m_1', \dots, m_{n'}'\}$ where $n' = n - 1$, $x_i' = x_{i-1}^*$, $m_i' = m_{i-1}^*/(1-m_1)$. This modified problem may again be solved analytically or numerically. In general, theoretical considerations are different in some respects from merely practical ones.

Appendix: Proof of Theorem 1

We need the following auxiliary result. Let us call a design ξ nondegenerate if $det M(\xi) \neq 0$.

Lemma 1. *A nondegenerate design ξ^* minimizes (7) for model (4) — (5) iff*

$$\max_{x\in[0,1]} \left[(1-x) f^T(x) M^{-1}(\xi^*) f(1)\right]^2 = f^T(1) M^{-1}(\xi^*) f(1). \tag{8}$$

In addition the maximum in the left hand side is achieved for all points of an optimal design (if it is nondegenerate).

Proof of **Lemma 1.** Since (7) has the form

$$tr L M^{-1}(\xi)$$

where $L = f(1) f^T(1)$, the assertion of the lemma follows from the equivalence theorem for linear optimal designs (Kiefer, 1974).

Next we prove that any optimal design is nondegenerate. Note that a design ξ is nondegenerate iff the number of its points $n \geq k+1$. Expanding $det M(\xi)$ by the Binet-Cauchy formula, and using the fact that Vandermonde's determinant $(x_j^{i-1})_{i.j=1}^k$ with $0 \leq x_1 < x_2 < \dots < x_{k+1}$ does not vanish proves the assertion.

If a design ξ is not degenerate then, by a well-known criterion (see, for example, Rao, 1966), $\theta^T f(1)$ is estimable iff

$$f(1) = \sum_{i=1}^{l} \alpha_i f(x_i)(1-x_i) \tag{9}$$

for some real numbers $\alpha_1, \ldots, \alpha_l$, where $l < k+1, x_i \le 1, i = 1, 2, \ldots, l$ are points of ξ.

Without loss of generality we can assume that $l = k, x_i < 1 (i = 1, 2, \ldots, l)$. Then from (8) it follows that

$$det \begin{Vmatrix} 1 & 1 - x_1 & \ldots & 1 - x_k \\ 1 & (1 - x_1)x_1 & \ldots & (1 - x_k)x_k \\ \ldots & \ldots & \ldots & \ldots \\ 1 & (1 - x_1)x_1^k & \ldots & (1 - x_k)x_k^k \end{Vmatrix} = 0$$

with $0 \le x_1 < x_2 < \ldots < x_k < 1$. However, the left hand side is equal to

$$\prod_{i=1}^{k}(1 - x_i)\prod_{i<j}(x_j - x_i) \ne 0.$$

The contradiction obtained shows that any optimal design is nondegenerate (otherwise $Var f^T(1)\hat{\theta} = \infty$).

Thus by Lemma 1 any optimal design ξ^* satisfies (8). Let $\xi^* = \{x_1^*, \ldots, x_n^*; \mu_1^*, \ldots, \mu_n^*\}$ be an optimal design. Since it should be nondegenerate, we have $n \ge k+1$. Define $b = M^{-1}(\xi^*)f(1), y = \sqrt{x}$.

In accordance with (7) the polynomial

$$P(y) = (1 - y^2)f^T(y^2)b$$

takes its maximal value at the points $\pm\sqrt{x_i^*}$, $x_i^* < 1, i = 1, \ldots, n, P(1) = 0$. Note that the degree of $P(y)$ is no more than $2k+1$, and $P(y) \not\equiv const$. The number of distinct points among $\pm\sqrt{x_i^*}, i = 1, \ldots, n$ equals either $2n$ or (if $x_1^* = 0$) $2n - 1$. Since $P(1) = 0$, $P(y)$ reaches its maximal value at $\pm\sqrt{x_i^*}, i = 1, \ldots, n$ and some points $\pm\sqrt{x^*}, x^* > 1$. ¿From this $2n \le 2k+1$ and since $n \ge k+1$ then $n = k+1$ and $x_1^* = 0$. It is well known (see, for example, Fedorov, 1972) that the Tchebysheff polynomial of first kind $T_{2k+2}(y)$ is the unique (with constant accuracy) polynomial which reaches its maximal absolute value on $[-1, 1]$ in $2k+3$ points. Therefore

$$P(y) = const T_{2k+2}(\tau y)$$

where $const = (f^T(1)M^{-1}(\xi^*)f(1))^{1/2}$, τ is the maximal root of $T_{2k+2}(y)$, and $x^* = 1/\tau$. Hence, the optimal design points should be $x_i^* = (y_i^*)^2/\tau^2$ where $y_i^* (i = 1, \ldots, k+1)$ are nonnegative extremal points of $T_{2k+2}(y)$ inside $[-1, 1]$. Thus

$$x_i^* = cos^2\left((i-1)\pi/(2k+2)\right)/\tau^2, \tau = cos(\pi/(4k+4)), i = 1, 2, \ldots, k+1.$$

The weights can be found in the following way. Consider the polynomial $Q(x) = f^T(x)b$. Let $L_i(x), i = 1, \ldots, k+1$ be the Lagrange interpolation polynomials associated with the points $x_1^*, \ldots, x_{k+1}^*$. Denote $C = f^T(1)M^{-1}(\xi^*)f(1) = Var f^T(1)\hat{\theta}/\sigma^2$. Then

$$Q(1) = f^T(1)b = C \quad \text{and} \quad Q(1) = \sum_{i=1}^{k+1} Q(x_i^*)/L_i(1).$$

By the Schwartz inequality, for arbitrary $\mu_i > 0, i = 1, \ldots, k+1$ we obtain

$$\begin{aligned} C^2 = |Q(1)|^2 &= \left|\sum_{i=1}^{k+1} \sqrt{\mu_i} Q(x_i^*)(1-x_i^*) \frac{L_i(1)}{(1-x_i^*)\sqrt{\mu_i}}\right|^2 \\ &\le \sum_{i=1}^{k+1} \mu_i Q^2(x_i^*)(1-x_i^*)^2 \sum_{i=1}^{k+1} \frac{L_i^2(1)}{\mu_i(1-x_i^*)^2}, \end{aligned}$$

and the equality holds iff $\mu_i = const|L_i(1)|/(1-x_i^*)$. Since $f^T(1)M^{-1}(\xi^*)f(1) = \min_\xi f^T(1)M^{-1}(\xi)f(1)$ and $Q^2(x_i^*)(1-x_i^*)^2 = C$, we obtain

$$\mu_i^* = \frac{|L_i(1)|/(1-x_i^*)}{\sum_{j=1}^{k+1} |L_j(1)|/(1-x_j^*)}, \quad C = \left|\sum_{j=1}^{k+1} L_j(1)/(1-x_j^*)\right|^2,$$

which completes the proof.

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No.	Author(s)	Title
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