

OPTIMIZATION OF SIMULATION RESPONSES IN A MULTICOMPUTING ENVIRONMENT

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This paper describes the application of experimental design techniques to computer simulation in a multicomputing environment. Three principal areas of experimental design are considered: (1) factor screening experiments; (2) experiments of comparison; and (3) response surface methodology.

INTRODUCTION

Simulation can be defined as the establishment of a mathematical-logical model of a system and the experimental manipulation of that model on a digital computer. This definition emphasizes two principal activities in computer simulation; (1) model development, and (2) experimentation. This paper concentrates on the second of these activities, and assumes that the simulationist has already developed a valid model of the system under study. We show how simulation experiments can be performed in a multicomputing environment.

The simulationist attempts to utilize the simulation model to gain an understanding of the relationships between a set of system responses

$$\eta_j = g_j(x_1, \dots, x_n), \quad j = 1, \dots, m \quad (1)$$

which are unknown to the simulationist. But by conducting a simulation trial at a point X^h using a set of random number streams S^h , where X^h is the p-vector of values (x_1, x_2, \dots, x_n) and S^h is the p-vector

of seeds $(S_1^h, S_2^h, \dots, S^h)$, the simulationist is able to observe a set of time series $\{y_j^h(t)\}$, $j = 1, \dots, m$, where $y_j^h(t)$ represents the measured value of j-th response variable η_j at time t for the h-th simulation trial. Unlike physical experimentation, which typically involves setting the values of the controllable factors at X^h and directly observing an m-vector of physical values Y^h , simulation requires a judicious selection of the initial seeds S^h for the random number streams that are used to generate the various random processes embedded in the model, as well as a choice of the duration of the trial. The duration is typically either (a) a fixed number of realizations N of a given response η_j , (b) a fixed period of simulated time T, or (c) the achievement of a specified state of the system. The experimental design procedures discussed in this paper are generally applicable to any of these three approaches for choosing the duration of the simulation.

Now the observed value y_j of a given system response η_j as a result of a simulation trial has the form

$$y_j = g_j(x_1, x_2, \dots, x_n) + \varepsilon_j, \quad j = 1, \dots, m \quad (2)$$

where ε_j has mean $E(\varepsilon_j) = 0$ and variance $\text{Var}(\varepsilon_j) = \sigma_j^2$. That is,

$$y_j = \eta_j + \varepsilon_j, \quad j = 1, \dots, m \quad (2a)$$

Now y_j actually represents the mean of a time series of realizations $\xi_{j\ell}$, $\ell = 1, \dots, r_j$, where r_j is the number of such realizations recorded during the simulation. That is,

$$y_j = \frac{1}{r_j} \sum_{\ell=1}^{r_j} \xi_{j\ell} \quad j = 1, \dots, m \quad (3)$$

The variance of this time series can be estimated by the relation

$$s_j^2 = \frac{1}{(r_j - 1)} \left[\sum_{\ell=1}^{r_j} \xi_{j\ell}^2 - r_j y_j^2 \right] \quad (4)$$

The estimates y_j and s_j^2 are unbiased estimates of η_j and σ_j^2 , respectively, where σ_j^2 is the true variance of the response η_j . If the succession of realizations $\xi_{j\ell}$, $\ell = 1, \dots, r_j$ are not independent, it is necessary to employ other formulae to compute the variance of this time series. Fishman (1978) discusses techniques for doing this.

In the following sections, we shall restrict our attention to a single system response η as a function of the n-vector of controllable factors x_i , $i = 1, \dots, n$.

A Multicomputing System

Before we can describe how simulation can be managed in a multicomputing environment, it is first necessary to describe that environment. A multi-computer is defined as a set of tightly coupled but autonomous computers, capable of synchronizing and communicating in parallel, and operating independently. Multicomputing requires a variety of unconventional software support tools including a powerful development operating system that can make use of the multicomputer's full capabilities, concurrent programming languages, debugging and concurrency simulation tools, a real-time operating system for parallel processing, and a self-diagnostic facility to monitor the activities of the entire system.

The Flex/32 Multicomputer provides a true Multiple Instruction Stream/Multiple Data System (MIMD) computing environment. It is a collection of 32-bit super minicomputers that share high-speed memory, intercomputer synchronization, and interprocess messaging hardware within a Multicomputing Environment. The Flex/32 Multicomputer can expand in

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processing power with minimal software modification and its hardware can be easily configured and reconfigured. Computer and/or memory cards can be added at any time to increase processing power. The configuration employed for this research has four 32-bit superminicomputers.

An autonomous computer has its own local bus, local memory, and Input/Output. This kind of Computing Element (CE) can operate independently or with other CE's as shown in Figure 1. This structure is called "multicomputing" and the Flex/32 Multicomputer is an example of such a system. The main advantage of having such a structure is that it satisfies the requirements for two distinct approaches of program decomposition. The first approach is one in which applications can be decomposed to individual processes, and where these processes can execute

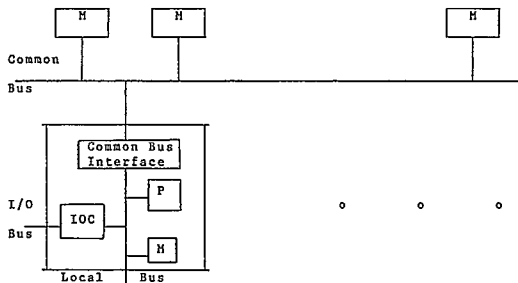


Figure 1: Flex/32 Multicomputer System Structure

independently for an extended period of time, between synchronization steps with other processes. This kind of decomposition, which is called "macro-level" decomposition, requires autonomous computers, having their own local memory blocks and local I/O's, in a tightly coupled environment. In the second approach, applications can also be decomposed down to their instruction level. In this type of application, blocks of instructions (such as loops, if-else's, et cetera) are divided into sub-blocks that can be executed by different computers. This "micro-level" type of decomposition requires a multiple processor system with a large common memory and a quick access of all processors to all common memory blocks.

The Flex/32 Multicomputer shown in Figure 1 provides a large common memory, while its processors are capable of operating independently by means of their local memory blocks and local I/O's.

The Flex/32 system provides a multicomputing environment by offering the following capabilities:

- UNIX System V as the development operating system,
- Concurrent languages such as Concurrent C, Concurrent Fortran, and Ada,
- A generic run-time support to provide multicomputing and real-time capabilities,
- Multicomputing Multitasking Operating System (MMOS) as a real-time OS,
- Concurrent UNIX Environment,
- Multicomputing development or execution support tools,

Simulation in a multicomputing Environment

Distributed simulation is the process by which large, complex simulation models are decomposed onto a set of processors. There are two major strategies by which this decomposition can be accomplished:

- Event decomposition in which each of the several events making up a model is assigned to a specific processor. This technique requires close time control and synchronization among the parallel processors. See Misra (1986)
- Task decomposition in which the various simulation functions such as I/O, event processing, random number and random variate generation, statistics collection, and report generation are allocated to different processors. See Wyatt and Sheppard (1984). This technique has the disadvantage that it requires a large degree of message passing, and thus invites the phenomenon known as "deadlock."

The procedure advocated here is simple in concept and overcomes the disadvantages brought on with either of the decomposition schemes mentioned above. Entire simulation runs are assigned to the individual processors, with only the experimental frames being different owing to the change in the input variables X and the random number streams S. The following sections describe how simulation is conducted for three main areas of statistical analysis and optimization:

- Factor screening
- Experimental designs
- Optimization methods

FACTOR SCREENING EXPERIMENTS

Of the n controllable factors in a computer simulation model, $k \leq n$ of these are also controllable in the real-world system. In addition to these, there is also a set of $n-k$ uncontrollable factors in the model that represent uncontrollable parameters in the real environment, but the simulationist is also interested in determining the response of the system to changes in these uncontrollable factors. For instance, in a model of a naval engagement, ship speed and rate of antimissile fire might be factors that are controllable by the commander in the real system, whereas weather effects and rate of enemy missile fire are factors beyond the commander's direct control. But the simulationist would attempt to measure the effects of each of these factors on the system response, which might be "probability of victory." In the simulation model, all of these factors would be controllable.

In general, not all of the n factors are equally important with respect to their effect on the response η . In factor screening, we attempt to isolate those factors which are highly important from those which are negligible. If $g < n$ factors exert important effects on η , we seek to have an experimental design indicate which factors these are. Jacoby and Harrison (1962) discuss these concepts. Smith and Mauro (1982) have produced an up-to-date treatment of this subject.

In factor screening, it is generally assumed that the relative importance of a set of n factors can be established by examining the coefficients β_i in the linear model

$$y = \beta_0 + \sum_{i=1}^n \beta_i x_i + \varepsilon \quad (5)$$

To perform an experiment with the simulation model, we perform simulation trials at each of a set of settings of X which involve one or more levels of each of the n controllable variables x_i , $i = 1, \dots, n$. The method of least-squares is then employed to estimate the main effects and interactions. From this analysis, the g most important factors are identified.

Some of the experimental designs employed in factor screening include the following:

- 2^n factorial experiments, involving a simulation trial at each of the $N = 2^n$ design points.
- 2^{n-p} fractional factorial designs, where n is large and 2^n simulations represent a very costly investment.
- Supersaturated plans, in which each of the n factors appears at high and low levels $N/2$ times, $N \leq n$.
- Groups screening designs, in which h groups of the n factors are identified, each such group is considered a single factor, and a 2^h factorial or 2^{n-p} fractional factorial design is employed to evaluate these group effects.

An important consideration in factor screening is that of variance reduction. Because simulation produces a times series of realizations ξ_{ℓ} , $\ell = 1, \dots, r$ for the response η , where the time series is induced by a series of pseudorandom numbers, it is possible to reduce the variance of the time series by judicious selection of these pseudorandom numbers. Two well-known variance reduction techniques are as follows:

- Common pseudorandom numbers, where the same set of initial random number seeds S are employed for each simulation trial in the designed experiment.
- Antithetic pseudorandom numbers, where the series of random numbers for one stream R' is the complement of another stream R; that is $r' = 1 - r$ for each successive pseudorandom number.

Schruben and Margolin (1978) describe a very useful technique for pseudorandom number assignment in simulation experiments to achieve variance reduction.

EXPERIMENTS OF COMPARISONS

Some of the n controllable factors are such that they assume quantitative levels in the experiments design. For example, ship speed and rate of anti-missile fire are quantitative variables which can be set at selected levels over a continuum of values $a_i \leq x_i \leq b_i$. Other controllable factors are definitely qualitative in nature. For example, the sea state could be calm, high seas, or stormy. In many simulation situations, the simulationist seeks to compare the response η at one level of a controllable factor to that at a different level. Such evaluations are called "experiments of comparison." The controllable variables in such experiments are called factors, and the different levels of each factor are called treatments.

The principal experimental designs employed with experiments of comparison are as follows:

- 2^n factorial designs, as discussed by Biles and Swain (1980) or Montgomery (1976).
- 2^{n-p} fractional factorial designs, as discussed by Box and Hunter (1961).

These designs are illustrated in Figure 2.

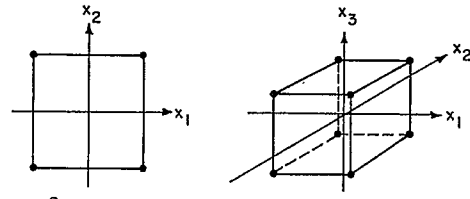


FIGURE 2. 2^n FACTORIAL DESIGNS

Biles and Swain (1980) discuss analysis of variance procedures by which the simulation results obtained from factorial designs are evaluated. These techniques enable the simulationist to test the null hypotheses that the individual factors exert no influence on the behavior of the system response η , or that two-factor interactions exert no effects. As with the factor screening experiment, it is necessary to adopt either common pseudorandom numbers or antithetic pseudorandom numbers to minimize the variance of the estimates.

RESPONSE SURFACE METHODOLOGY

Factor screening and experiments of comparison are not the only objectives the simulationist might have with respect to simulation experimentation. Often it is necessary to utilize the simulation model to attempt to find the optimum conditions for operating the system. These optimum conditions are here denoted as X^* and η^* .

The body of techniques by which one experimentally seeks an optimum set of system conditions is called response surface methodology. The following sections describe first and second order response surface methods as they relate to simulation experimentation.

First-Order Response Surface Methods

First-order response surface methods attempt to accomplish experimentally what the "method of steepest ascent" accomplishes computationally. From a current point X^k , a designed experiment is conducted (with a simulation trial at each design point) to estimate the gradient direction $\nabla g(X^k)$. Simulation trials are then conducted at points along this direction to a new point X^{k+1} which represents the best solution obtained along the direction $\nabla g(X^k)$. This process is an experimental approximation of the relation

$$X^{k+1} = X^k + \lambda^k [\nabla g(X^k)] \quad (6)$$

The step length λ^k can be estimated by a line search or by a regression procedure as described by Biles and Swain (1979).

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The gradient direction $\nabla g(X^k)$ is estimated by placing an appropriate first-order experimental design, such as a 2^n factorial, 2^{n-p} fractional factorial, or n -dimensional simplex design around the current point X^k . A simulation trial is performed at each point in the selected experimental design. From these N observations the multiple linear regression model

$$\hat{y} = b_0 + \sum_{i=1}^n b_i x_i \quad (7)$$

can be estimated. Since the gradient direction $\nabla g(X^k)$ is mathematically defined as the n -vector of first partial derivatives of $g(X)$ evaluated at X^k , it is clear that $\nabla g(X^k)$ is simply the n -vector of regression coefficients, exclusive of the b_0 term; that is,

$$\nabla g(X^k) = (b_1, \dots, b_n)' \quad (8)$$

In the multiple-response simulation problem, a simulation trial is conducted at each design point in the selected first-order design and the m observations y_j , $j = 1, \dots, m$ are recorded at each design point. Multiple linear regression is applied separately to each set of observations (assuming independence among the m responses), producing the m models

$$\hat{y}_j = b_{j,0} + \sum_{i=1}^n b_{j,i} x_i, \quad j = 1, \dots, m \quad (9)$$

and hence the m gradient vectors

$$\nabla g_j(X^k) = (b_{j,1}, \dots, b_{j,n})', \quad j = 1, \dots, m \quad (10)$$

These estimates can then be employed in any one of several optimization schemes to produce an improved solution X^{k+1} . A generalized procedure for accomplishing this improved solution, and an estimated "optimum," will be described later. But first it is necessary to give attention to the experimental designs employed to estimate the gradient vectors $\nabla g_j(X^k)$, $j = 1, \dots, m$.

In selecting a first-order response surface design, it is usually desirable to minimize the variances of the regression coefficients b_i , $i = 1, \dots, n$. To accomplish this the first-order experimental design should be orthogonal. An orthogonal first-order experimental design is constructed as follows: The placement of the N experimental points (in our case, simulation trials) is described by the N by n design matrix D , where

$$D = \begin{bmatrix} x_{11} & x_{21} & \cdots & x_{n1} \\ x_{12} & x_{22} & \cdots & x_{n2} \\ \cdot & \cdot & \cdot & \cdot \\ x_{1N} & x_{2N} & \cdots & x_{nN} \end{bmatrix} \quad (11)$$

An N by $n+1$ matrix X is then formed by placing a unit vector to the left of D . Thus

$$D = \begin{bmatrix} 1 & x_{11} & x_{21} & \cdots & x_{n1} \\ 1 & x_{12} & x_{22} & \cdots & x_{n2} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & x_{1N} & x_{2N} & \cdots & x_{nN} \end{bmatrix} \quad (12)$$

It is usually convenient to code the levels, design so that the following conditions are achieved:

$$\left. \begin{aligned} \sum_{u=1}^N x_{iu}^2 &= N \\ \sum_{u=1}^N x_{iu} &= 0 \end{aligned} \right\} \quad i = 1, \dots, n \quad (13)$$

If the actual value of the u -th level of the i -th variable is z_{iu} , then the corresponding coded value is

$$x_{iu} = \frac{z_{iu} - \bar{z}_i}{S_i} \quad (14)$$

where

$$\bar{z}_i = \left\{ \sum_{u=1}^N z_{iu} \right\} / N \quad (15)$$

and

$$S_i = \left\{ \sum_{u=1}^N (z_{iu} - \bar{z}_i)^2 \right\} / N \quad (16)$$

Then

$$X'X = \begin{bmatrix} N & 0 & 0 & \cdots & 0 \\ 0 & N & 0 & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdots & N \end{bmatrix} \quad (17)$$

Since the $(n+1)$ -vector of regression coefficients \bar{b} is estimated by the least squares relation

$$\bar{b} = (X'X)^{-1} X' \bar{y} \quad (18)$$

where \bar{y} is the N -vector of response estimates obtained from N simulation trials. The variance of the regression coefficients b_i , $i = 1, \dots, n$ is given by

$$\text{Var}(b_i) = \sigma^2 / N, \quad i = 1, \dots, n \quad (19)$$

where σ^2 is the variance of the error term ε . Since we are interested in m separate system response y_j , $j = 1, \dots, m$ equations (18) and (19) can be generalized to

$$\bar{b}_j = (X'X)^{-1} X' \bar{y}_j, \quad j = 1, \dots, m \quad (20)$$

$$\text{Var}(b_{ji}) = \sigma_j^2 / N, \quad i = 1, \dots, n; \quad j = 1, \dots, m \quad (21)$$

Again, with the coding scheme in (14), equation (20) simplifies to $b_i = n^{-1} X^T y_i$. For an orthogonal first-order design, the results in (17)-(21) hold, giving a so-called "minimum-variance" design. The 2^n factorial and 2^{n-p} fractional factorial designs are orthogonal and hence minimum variance. Orthogonal n-simplex designs can be easily constructed. Since n-simplex designs provide the minimum number of design points needed to estimate the multiple-linear regression models in (7) or (9), and are hence the most "economical" of the first-order response surface designs, they are especially attractive for the purpose proposed here. Figure 3 illustrates n-simplex designs.

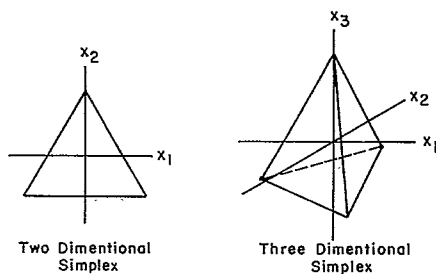


FIGURE 3. n-SIMPLEX DESIGNS

Biles and Swain (1979) have described a first-order response surface procedure for approaching the constrained formulation of the multiple-response simulation problem. This procedure involves performing a first-order design around a current point X^k to estimate the gradient direction $Vg(X^k)$ according to relation (8). A line search is then performed along $Vg(X^k)$ to estimate an optimal step λ in (6). As long as the search remains interior to the region bounded by the constraints, the procedure is basically a gradient search. If one or more constraints are encountered, however, Biles and Swain (1979) propose that the gradient projection direction be followed. The procedure for estimating the gradient projection direction is as follows.

Suppose that at an estimated boundary point X^k , q constraints are satisfied as equalities. Let B be the $n \times q$ matrix of first partial derivatives of q these active constraints. Thus, B consists of the q gradient vectors $Vg_j(X^k)$, $j = 1, \dots, q$. This is

$$B_q = \begin{bmatrix} \partial g_1 / \partial x_1 & \dots & \partial g_q / \partial x_1 \\ \vdots & & \vdots \\ \partial g_1 / \partial x_n & \dots & \partial g_q / \partial x_n \end{bmatrix} \quad (22)$$

Since $g_j(X)$, $j = 1, \dots, q$ denotes the set of binding constraint functions, for the moment let $f(X)$ represent the objective function. The $Vf(X^k)$ and $Vg_j(X^k)$, $j = 1, \dots, q$ represent the gradient vectors of the objective and constraint functions, respectively, evaluated at the boundary point X^k .

Performing a first-order response surface experiment about the boundary point X^k yields estimates of the gradient vectors $Vf(X^k)$ and $Vg_j(X^k)$, $j = 1, \dots, q$ in the form of the vectors of regression coefficients. The gradient projection direction is then given by

$$S^k = [Vf(X^k)] - B_q (B_q^T B_q)^{-1} B_q^T [Vf(X^k)] \quad (23)$$

A line search is performed along direction S^k until either (a) a local "optimum" is found, or (b) other constraints are encountered. This new point is denoted X^{k+1} . This procedure is repeated until the gradient projection direction S^k is approximately zero. This point X^* is taken as a "constrained optimal" solution. Figure 4 illustrates the application of the gradient projection procedure to a constrained optimization problem.

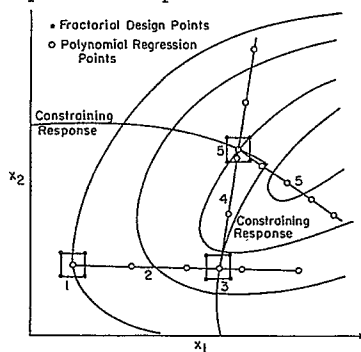


FIGURE 4. FIRST-ORDER RESPONSE SURFACE OPTIMIZATION

The following generalized procedure is followed in employing a first-order response surface approach to the multiple-response simulation problem. The particular problem formulation and optimization procedure will govern the precise sequence of steps in implementing this procedure.

1. Identify the known experimental region $a_i \leq x_i \leq c_i$, $i = 1, \dots, n$. Select a starting point X^0 within this region. With X^0 as its center, array an orthogonal first-order response surface design within a selected design radius. Place $n_0 = n/2 \geq 2$ points at the design center X^0 (coded as the 0-vector).
2. Perform simulation trials at each of the N experimental design points and record the responses y_j , $j = 1, \dots, m$; $\ell = 1, \dots, N$. Using multiple linear regression, fit linear models of the form (9).
3. Apply the appropriate mathematical programming technique to locate the next center point in the search.
4. Repeat steps 1-3 until an "optimum" solution is located. It may be appropriate to add design points to complete a second-order response surface design to test this optimum solution. The procedure for accomplishing this is described in the next section.

Second Order Response Surface Methods

A second-order response surface approach to the multiple-response simulation problem consists of one or more repetitions of a two-stage procedure: (a) the execution of a computer simulation trial at each point in a second-order response surface experimental design covering the known experimental region, and the use of multiple linear regression to fit second-order regression models to the resulting data; and (b) the application of a suitable mathematical programming procedure to obtain a solution to the resulting optimization problem. In contrast to the first-order methods, in which the optimization proce-

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cedure was part and parcel with the experimental procedure, these procedures are distinct and sequential in the proposed second-order approaches.

The first step in the second-order approach is to identify the range of each input variable. A safe strategy is to cover the entire known region $a_i \leq c_i$, $i = 1, \dots, n$ with the first (and possibly only) experimental design. If we let α_i denote the radius of the n -dimensional hypersphere within which the design points are contained, then

$$\alpha_i = (c_i - a_i)/2, \quad i = 1, \dots, n \quad (24)$$

is effectively the maximum radius we could construct. It is convenient to adopt the coding convention expressed in (14)-(16), but choosing x_{ij} in such a way that α_i satisfied (24). Biles and Swain (1980) describe this coding process.

The second-order fitted response surface has the form

$$\hat{y} = b_0 + \sum_{i=1}^n b_i x_i + \sum_{i=1}^n b_{ii} x_i^2 + \sum_{i=1}^n \sum_{j=1}^n b_{k,ij} x_i x_j \quad (25)$$

$i \neq j$
 $k = 1, \dots, m$

where \hat{y} is the estimate of the true response η at a given value $X = (x_1, \dots, x_n)$ and the b_i and b_{ij} are regression coefficients in the fitted model. Since we must estimate m separate response relationships, equation (25) is modified to

$$\hat{y}_k = b_{k,0} + \sum_{i=1}^n b_{k,i} x_i + \sum_{i=1}^n b_{k,ii} x_i^2 + \sum_{i=1}^n \sum_{j=1}^n b_{k,ij} x_i x_j \quad (26)$$

$i \neq j$
 $k = 1, \dots, m$

Given the independence of the m responses, these m regression equations can be estimated independently from a set of $N \geq (n+1)(n+2)/2$ data points obtained by performing a simulation trial at each point in a second-order response surface design.

An experimental design employed for the purpose of estimating the regression coefficients in (26) must contain at least as many design points as there are coefficients b_i and b_{ij} in the fitted model, of which there are $(n+1)(n+2)/2$. Because of the non-linearity of (26), the experimental design must also have at least three levels of each controllable variable x_i , $i = 1, \dots, n$. It is also desirable to have a design which is rotatable; that is, the predicted response y at some point X is a function only of the distance from the design center to X and not a function of the direction.

The most widely used design for fitting a second-order model is the central composite design, shown in Figure 5 for $n=2$ and $n=3$. These designs consist of a 2^n axial points and k center points. A central composite design can be made rotatable by proper choice of α , the distance of the axial points from the design center. With the proper choice of the number of center points k , the central composite design can be made either orthogonal or uniform precision.

Having estimated the m second-order regression equations (26) and formulated the appropriate optimization problem, it remains to apply mathematical programming to obtain a solution. For the constrained formulation, any of the following procedures could be employed: (a) Box's complex search; (b) Rosen's gradient projection method; or (c) one of Zoutendijk's methods of feasible directions. These are described in Biles and Swain (1980).

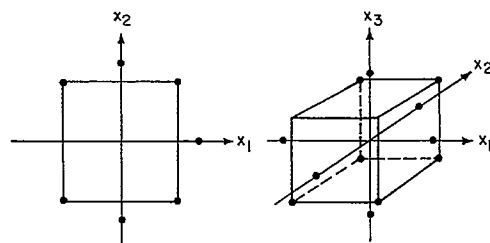


FIGURE 5. CENTRAL COMPOSITE DESIGNS

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