Journal of Probability and Statistical Science
1(1), 65-88, Feb. 2003

Using a Genetic Algorithm to Generate Small Exact Response Surface Designs

John J. Borkowski
Montana State University

ABSTRACT A genetic algorithm (GA) is an evolutionary search strategy based on simplified rules of biological population genetics and theories of evolution. A GA maintains a population of candidate solutions for a problem, and then selects those candidates most fit to solve the problem. After the selection process, the most fit candidate solutions are combined and/or altered by reproduction operators to produce new solutions for the next generation. The process continues, with each generation evolving more fit solutions until an acceptable solution is evolved. In this research, a GA is developed to generate near-optimal *D*, *A*, *G*, and *IV* exact *N*-point response surface designs in the hypercube. The optimal exact designs can be found by applying a local search algorithm to these near-optimal designs. A catalog of designs is given for 1, 2, and 3 design factors. Efficiencies are calculated for classical response surface designs relative to exact optimal designs of the same design size.

Keywords：Genetic algorithms; Response surface designs; Design optimality.

□Received June 2002, revised September 2002, in final form November 2002.
□John J. Borkowski is Associate Professor, Department of Mathematical Sciences, Montana State University, Bozeman, Montana 59717, USA; email: umsfjbor@math.montana.edu.

1. Introduction

In many research projects, experiments are run to describe relationships between design variables $x_1, x_2, \ldots, x_k$ and the response y of interest. In many industrial situations, a response surface design is implemented that will enable the experimenter to fit a second-order polynomial model:

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{j=i+1}^{k} \sum_{i=1}^{k-1} \beta_{ij} x_i x_j + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \epsilon. \quad (1)$$

where the β's are the parameter coefficients, y is the measured response and ϵ is an error term which accounts for random error and the deviation between the true model η and second-order polynomial.

In view of the high cost of collecting data in many investigations, particularly in experiments in industrial settings, keeping the design size manageable is a critical consideration. In such cases, the search for small, efficient designs becomes necessary and *design optimality criteria* are often used to evaluate and compare designs.

The *approximate theory* of optimal design which treats experimental designs as probability measures was developed by Kiefer and his colleagues (e.g. Kiefer [17-19], Kiefer and Wolfowitz [20], and Farrell, Kiefer, and Walbran [6]). Approximate theory ignores the practical constraint of implementablity, that is, the number of trials corresponding to any design point must be an integer. Any design for which the number of trials is a specified integer N is called an *exact design*. By definition, all implementable designs used by experimenters are exact.

An N-point response surface design is represented by an $N \times k$ design matrix. Each of the N rows corresponds to an experimental point whose k column entries are the experimental settings of the k factors. This design is expanded into an $N \times p$ *expanded design matrix* X where p is the number of model parameters. $p = \binom{k+2}{2}$ for the model in (1).

When an exact N-point design is being considered for implementation, the D, A, G, and IV design optimality criteria are often used for design evaluation. For each criterion, the optimization goal can also be expressed as an equivalent maximization goal:

Criterion	Optimize	Maximize
D	$d(X) = \lvert X'X \rvert$	$D(X) = 100 \lvert X'X \rvert^{1/p}/N$
A	$a(X) = \text{trace}\left[(X'X)^{-1}\right]$	$A(X) = \frac{100p}{\text{trace}[N(X'X)^{-1}]}$
G	$g(X) = \max_{x \in \mathcal{X}} \left[Nx'(X'X)^{-1}x\right]$	$G(X) = \frac{100p}{\max_{x \in \mathcal{X}}[Nx'(X'X)^{-1}x]}$
IV	$i(X) = (1/V) \int_{\mathcal{X}} Nx'(X'X)^{-1}x \;\; dx_1 \ldots dx_k$	$I(X) = \frac{V}{\int_{\mathcal{X}} Nx'(X'X)^{-1}x \;\; dx_1 \ldots dx_k}$
	$= \;\; (N/V)\text{trace}[W(X'X)^{-1}]$	$= \frac{V}{N\text{trace}[W(X'X)^{-1}]}$

where $x' = [f_1, \ldots, f_p]$ is a vector of p real-valued functions of $(x_1, \ldots, x_k)$ based on the model terms, V is the volume of the design space $\mathcal{X}$, and $W = \int_{\mathcal{X}} xx' dx_1 \ldots dx_k$. For the second order model in (1), $x' = (1, x_1, \ldots, x_k, \; x_1x_2, \ldots, x_{k-1}x_k, \; x_1^2, \ldots, x_k^2)$. In this research, $\mathcal{X}$ will represent the design space where the minimum and maximum levels of each of the k design factors are scaled to be ± 1. That is, $\mathcal{X}$ is restricted to the k-dimensional hypercube $[-1, 1]^k$ with $V = 2^k$. The G and IV criteria respectively correspond to minimizing the maximum and minimizing the average scaled prediction variance over all points $x \in \mathcal{X}$. For a detailed discussion of optimal design criteria, see Atkinson and Donev [1].

To calculate a design's D, G, A, or IV *efficiency*, the theoretical maximum of $D(X)$, $A(X)$, $G(X)$, or $I(X)$, denoted, D_{opt}, G_{opt}, A_{opt}, and I_{opt}, must be found. Design efficiencies are

$$D_{eff}(X) = \frac{D(X)}{D_{opt}} \qquad A_{eff}(X) = \frac{A(X)}{A_{opt}} \qquad G_{eff}(X) = \frac{G(X)}{G_{opt}} \qquad IV_{eff}(X) = \frac{I(X)}{I_{opt}}$$

If an experimenter, however, wants to compare several N-point designs, it would be appropriate to compare $D(X)$, $A(X)$, $G(X)$, or $I(X)$ to the corresponding value of an *optimal exact* N-point design. Let D^N_{opt}, G^N_{opt}, A^N_{opt}, and I^N_{opt} be the maxima of $D(X)$, $A(X)$, $G(X)$, and $I(X)$ when taken over all possible exact N-point designs. By looking at *relative design efficiencies*

$$D^N_{eff}(X) = \frac{D(X)}{D^N_{opt}} \qquad A^N_{eff}(X) = \frac{A(X)}{A^N_{opt}} \qquad G^N_{eff}(X) = \frac{G(X)}{G^N_{opt}} \qquad IV^N_{eff}(X) = \frac{I(X)}{I^N_{opt}} \quad (2)$$

the experimenter can gauge how good his/her N-point design is relative to all possible N-point designs based on that optimality criterion.

Table 1 summarizes the limited number of designs that are claimed to be optimal exact. For the * cases, the author could not find a design in a publications search. If the entry includes $>$, it indicates that a slightly better design was found using a GA. Table 1 indicates that (i) many new exact designs were generated and (ii) the designs generated by the GA are either identical to or are slightly better than the 1 and 2 factor designs generated by simulated annealing (Haines [11]), the designs generated by the IV-algorithm of Crary et al. [4], as well as those recorded in Atkinson [1] and Box and Draper [2].

Currently, we do not know how good any N-point design is relative to an optimal exact N-point design. For example, suppose a software package generates an N-point design based on maximizing the D or A criterion (e.g., the *Optex* procedure in *SAS* (SAS Institute [26]). Because it was formed from a finite set of candidate points it is very unlikely that this design is the optimal exact design. Also, the design-generating algorithms of Wynn [30], Federov [7], Mitchell [24], Welch [28, 29] are based on optimizing the D-criterion over a discrete set of candidate points.

In k-dimensional continuous design regions such as the hypercube, finding an optimal exact N-point design is computationally complex. It involves finding a total of $N \times k$ design variable settings that will optimize $D(X)$, $A(X)$, $G(X)$, or $I(X)$ and which will have numerous local optima. This is when a GA will be useful. With a GA, all points in the hypercube are potential design points, thereby circumventing the limitations imposed by discretization of the hypercube required for the existing algorithms. The GA will lead to the generation of near-optimal D, G, A, and IV exact N-point designs. The optimal exact designs can be found by applying a local search algorithm to these near-optimal designs.

2. Genetic Algorithms

A genetic algorithm is an evolutionary search strategy based on simplified rules of biological population genetics and theories of evolution. A genetic algorithm (GA) maintains a

population of candidate solutions for a problem, and then uses a biased sampling procedure to select the solutions that seem to work well for the problem (that is, optimizing an objective function). After this selection process, the most fit candidate solutions are combined or altered by "reproduction" operators to produce new solutions for the next generation. The process continues, with each generation evolving more fit solutions until an acceptable solution has evolved.

The foundations of GAs were developed by John Holland in the 1960s and are detailed in Holland [16]. In the mid 1980s, GAs were adopted by disciplines outside the artificial intelligence community. For example, GAs have provided solutions to complex problems in optimization, machine learning, programming, and job scheduling. See Michalewicz [22] and Haupt and Haupt [14] for an introduction to GAs. Greffenstette [10], Schaffer [27], Davis [5] and Michalewicz [23] provide applications of GAs across many disciplines. GAs are attractive not only because they are relatively easy to implement, but mathematically they do not require a differentiable objective function and they reduce the chance of reporting local optima.

The GA terminology originates from biology and computer science sources. Familiarity with the GA terminology is integral in the presentation of this research and will now be presented.

3. Genetic Representation and the Objective Function

For any GA, the construction of the genetic representation of a chromosome is required. A **chromosome** represents a potential solution to the problem of interest and traditionally is represented by a string of **genes** that are either *binary encoded* or *real-number encoded*. In a real number representation, genes are encoded with real numbers while in a binary representation, genes are encoded 0 or 1. In practice, Davis [5] has found that GAs using real number representations have out-performed GAs with binary representations in numerical optimization problems. This is also the opinion given in Haupt and Haupt [14]. Because real number representation works effectively on mathematical optimization problems and allows for the use of numerical reproduction operators, it will be used in this research. For an introduction to real number representations, see Goldberg [8], Davis [5] and Michalewicz [22]. Theory regarding the performance of GAs with real number representations is developed in Goldberg [9].

The **objective function** F measures a chromosome's *fitness* as a solution and is the function we wish to optimize. F takes a chromosome as input and outputs an objective function value.

The research goal is to develop a GA that will generate exact N-point k-variable response surface designs. Equivalently, the goal is to find an $N \times k$ matrix that optimizes a design optimality criterion. Chromosomes, genes, and the objective function will now be redefined in terms of an experimental design and design optimality criteria. A **chromosome** C is an $N \times k$ matrix representing the N design points in k factors. When C is expanded to include columns

for all the p terms in the model, it yields the $N \times p$ expanded design matrix X. A **gene** is any of the $N \times k$ real-number x_{ij} entries in the chromosome C. That is, x_{ij} is the coded setting of the i^{th} factor in the j^{th} experimental run. A gene's value is dictated by the design region $\mathcal{X}$. In this case, each $x_{ij} \in [-1, 1]$.

Because designs will be evaluated using the D, A, G, and IV criteria, four **objective functions** will be used. The goal is to evolve a design that maximizes an objective function F_i where

$$F_D = D(X) \qquad F_A = A(X) \qquad F_G = G(X) \qquad F_I = I(X).$$

F_i measures C's fitness as a solution in the search for an exact design relative to criterion i.

4. Selection and Reproduction

In the **selection process**, the GA selects chromosomes with superior fitness relative to the existing population so their good traits can be passed on to future generations of chromosomes and, therefore, does not allow inferior chromosomes to reproduce. In other words, the success of the GA is based on a 'survival of the fittest' biological imperative. Although there are many methods for selecting chromosomes for the reproduction process (e.g., see Michalewicz [22]), Haupt and Haupt [14]), the following simple approach was adopted:

I. At the beginning of every generation the population consists of an even number M chromosomes (designs). The two best or *elite* chromosomes (based on the objective function) are retained and left unchanged. The remaining $M - 2$ chromosomes are randomly partitioned into $(M - 2)/2$ pairs of *parent chromosomes*.

II. Each of these $(M - 2)/2$ parental pairs reproduces. After the reproduction process is completed there is an *offspring chromosome* associated with each parent. Thus, there are the 2 elite, $M - 2$ parent, and $M - 2$ offspring chromosomes for a total of $2M - 2$ chromosomes at the end of a reproduction cycle.

III. The objective function F_i values are calculated for the $2M - 2$ chromosomes. For each parent-offspring pair, the chromosome with the better F_i value survives to be a future parent and the other is removed from the population. Thus, at the end of every generation, $M - 2$ future parent chromosomes and the 2 current elite chromosomes survive to the next generation. These M chromosomes are then sorted and the two with the best F_i values become the elite for the next generation.

For example, suppose we are trying to generate a D-efficient design and there are 16 designs in the population. There are 2 elite designs having the highest D-criterion values, leaving 7 random pairs of designs to be formed. Reproduction proceeds for the 7 parental design pairs yielding 14 offspring designs. The objective function F_D is calculated for the two elite designs and each of the 14 parent-offspring pairs of designs. The two elite designs and the designs having the larger F_D within each of the 14 parent-offspring pairs survive to the next generation.

The **reproduction process** will operate on the genes (factor settings) to produce offspring chromosomes. A gene changes (i.e., evolves) if a **probability test** is passed. In this research, a probability test is a Bernoulli trial with probability of success α. Let u be a random deviate from a $[0, 1]$ uniform distribution. If $0 \leq u \leq \alpha$ then the probability test is passed (PTIP) and the reproduction operator is applied. If $\alpha < u \leq 1$ then the probability test is not passed and the chromosome is left unchanged.

The *blending, creep*, and *elitism* reproduction operators and three new operators called *sign change*, *zero gene* and *extreme gene* will be used. All of these reproduction operators except elitism requires a probability test. The success probabilities for the blending, creep, sign change, zero gene, and extreme gene operators are, respectively, $\alpha_b, \alpha_c, \alpha_s, \alpha_z$, and α_e. Choices for these α_i will be discussed in Step 5 in Section 5.

Let A and B be two parents paired in the reproduction process. A PTIP is applied to each row of A. Let A_a be the a^{th} row of A. If a PTIP for A_a, the **blending** operator will combine A_a with a random row of B, say B_b, to form two new rows: A_a^* and B_b^* via the linear combinations:

$$A_a^* \;=\; \beta A_a \;+\; (1-\beta)B_b \qquad \text{and} \qquad B_b^* \;=\; \beta B_b \;+\; (1-\beta)A_a$$

where β is a random $[0, 1]$ uniform variate.

For the **creep** operator, if a PTIP, a random variate ϵ from a normal $N(0, \sigma^2)$ distribution is added to a gene x_{ij} to form a new gene $x_{ij}^* = x_{ij} + \epsilon$. If the creep operator takes $x_{ij}^* > 1$ or $x_{ij}^* < -1$ it will be reset to the boundary value $x_{ij}^* = \pm 1$. The variance σ^2 is set by the researcher. For the **sign change** operator, if a PTIP for x_{ij}, the sign of the gene is changed. That is, we replace x_{ij} with $-x_{ij}$. For the **zero gene** operator, if a PTIP, a gene x_{ij} is set to 0. For the **extreme gene** operator, if a PTIP, a gene x_{ij} is randomly set to either ± 1. For these four gene operators, a PTIP is applied to every gene x_{ij} of each parent chromosome in the reproduction process. Because the operator sweeps through all of the chromosome's genes, different subsets of the $N \times k$ entries in a design C can be modified. These operators allow exploration of the design space (in particular, near the center and on the boundary of the hypercube), reduce the chance of being trapped at a local optimum, and let evolution to a superior design proceed rapidly.

Elitism retains the best chromosomes from the present generation which guarantees that the most fit chromosomes that have evolved thus far will survive to the next generation. In this research, the 2 best or 'elite' designs are retained but are not allowed to participate in the reproduction process until some future chromosome with better fitness evolves to take their place.

In the GA, probability tests were implemented in the following order: blending, zero gene, extreme gene, sign change, and creeping. Operators will be applied multiple times per generation when more than one PTIP. This will ensure a diversity of changes during the reproduction process, especially, when the creep operator is last. Note: the order proposed is based on the

best judgment of the author. Although this may not be optimal in terms of minimizing the number of generations to achieve the best designs, it will not prevent convergence. The optimal ordering of operators is an open area of research.

5. The Five Steps of the GA

Suppose F_i is the objective function selected for the GA. The GA used in this research can be summarized in five steps. All computation was performed using author-written programs for Matlab computational software (The MathWorks [21]).

1. *Create an initial population of M chromosomes.* Because all good response surface designs have space-filling properties (that is, each of the 2^k quadrants of the k-dimensional hypercube should contain design points), the number of points in each quadrant were allocated as equally as possible. For example, if $k = 2$ and $N = 11$, then 3 quadrants have 3 points and 1 quadrant has 2 points. Points are then randomly selected in each quadrant. N points could be randomly selected in the hypercube to create an initial design, but a much larger number of generations may be required for the population to evolve a good design. Although we would want a large M, choice of M was based on practical computing time considerations. Increasing M reduces the chances of reporting a local optimum.
2. *Use F_i to evaluate the fitness of each of the M chromosomes* in the initial population. The two designs having the largest F_i values will be the elite designs. When $F_i = F_G$, the estimate of F_G is the maximum of $G(X)$ over the 5^k points where each coordinate $x_j \in \{0, \pm.5, \pm1\}$ for $j = 1, \ldots, k$.
3. *Create offspring chromosomes by mating chromosomes.* Mating occurs by applying the operators in the order described in Section 4 row-by-row for each parent pair when a PTIP. F_i is calculated for each parent/offspring pair, and the more fit chromosome (larger F_i) in the pair is retained for the next generation while the other is removed. The reproduction process will yield the next generation of M designs (2 elite and $M - 2$ future parents).
4. *Iterate the selection and reproduction process.* That is, apply step 3 for a large number of generations. Respectively, 12000, 18000, and 21000 iterations were used to generate designs for 1, 2, and 3 factors. The α_i success probabilities were reset to new values after 6000 iterations. Because there are no rules for selecting the α_i values and the choice of the α_i values affects the speed of convergence to the optimal design, the levels were varied during multiple runs of the GA for a fixed N and optimality criterion. The following summarizes the ranges of α_i values: $0 \le \alpha_e, \alpha_s, \alpha_z \le .20$ and $.01 \le \alpha_c, \alpha_b \le .20$. Larger α_i values were used for the early iterations and smaller α_i values were used for the later iterations. Also, $.001 \le \sigma \le .10$, for the creep operator standard deviation. Like the α_i, larger σ values were used for the early iterations and smaller values were used for the later iterations. Choice of each α_i was based on the judgment of the author and is not optimal. Choice of α_i, like the order of operators, is an open research area.

5. *Report the chromosome with the largest fitness value.* After the final iteration, a local grid search is applied to the points of the design with the largest F_i value. If $F_i = F_G$, F_G is modified to be the maximum of $G(X)$ over the grid of 21^k points (instead of 5^k points) to improve accuracy. Because the majority of the most fit designs suggest symmetry, a constrained local grid search requiring the design to possess the symmetry structure was performed. For the six-point two-factor case, the most fit design based on F_D was $(-.1309, .1314), (1, -.3903), (.3990, -1), (1, 1), (-1, 1), (-1, -1)$ suggesting a structure of $(-a, a), (1, -b), (b, -1)$ for the first three points. The constrained local grid search found the best design to be $(-.1315, .1315)$, $(1, -.3944)$, $(.3944, -1)$, $(1, 1)$, $(-1, 1)$, $(-1, -1)$. The local grid search will increase the F_i value slightly until no further improvement can be found. This will be the reported optimal exact design.

Example: Consider the two factor case where the goal is to generate a D-optimal exact six point design and the initial population contains $M = 6$ chromosomes. In Step 1, six 6-point chromosomes (C1, C2, C3, C4, C5, C6) are generated. Table 2 is one possible realization of the initial population. In Step 2, F_D is evaluated for the 6 chromosomes. The values are given at the bottom of Table 2. Because C3 and C6 have the largest F_D values, they are the elite chromosomes.

In Step 3, C1, C2, C4, and C5 will be randomly paired for the reproduction process. Suppose (C4,C1) and (C2,C5) are the random pairs. The reproduction process for C4 and C1 will yield offspring C4* and C1*. Table 3 contains the random uniform deviates for the probability tests performed on C4 and C1. Boldfacing indicates the PTIP (i.e., the deviate $< \alpha$). Note that no PTIP is passed for the sign change operator. The following discussion of the first generation is summarized in Table 4 where boldfacing indicates a gene was changed.

Let x_{ij} and y_{ij} be the (i, j) genes in C4 and C1, respectively. Because the reproduction operators are applied row-by-row in the order blending $\rightarrow$ zero gene $\rightarrow$ extreme gene $\rightarrow$ sign change $\rightarrow$ creep, the first probability test passed is the creep operator on y_{12}. The randomly generated $\epsilon = -.2293$ which when added to y_{12} is $-.3530$. See Table 4 for the ϵ values. In row 2, no PTIP. Next, a creep PTIP for x_{31} and for y_{31} and random ϵ values are added. In row 4, x_{41} will be set to 0, y_{41} and y_{42} will be set to -1 and 1, respectively. Because a creep PTIP for x_{41} and y_{41}, their current values of 0 and -1 will be changed by a random ϵ.

The *Blend* column indicates row 5 of C4 = [.0087 .5591] will be blended with a random row of C1. Row 2 of C1 = [-.5576 .1673] was selected with random blending value $\beta = .3644$ yielding:

$$\begin{aligned} \text{Row 5 of C4}^* = \quad & .3644([.0087.5591]) + (1 - .3644)([-.4476.1673]) \quad = [\text{-}.2813\ .3101] \\ \text{Row 2 of C1}^* = \quad & .3644([-.4476.1673]) + (1 - .3644)([.0087.5591]) \quad = [\text{-}.1576\ .4163]. \end{aligned}$$

x_{51} and x_{52} are then set to 0 and y_{52} is set to -1. Next, row 6 of C4 = [.5813,.3015] is blended with the current row 5 of C1 = [.5551,-1] using random $\beta = .3542$. Finally, x_{61} is changed to 0 and then to 1. The offspring chromosomes that evolved are given at the end of Table 4.

Note: In Table 4 there are two row 2 and two row 5 pairs in the *After Blending* columns. The upper pair indicate that these values were not initially changed when performing the probability tests in rows 2 and 5. The lower pair of values indicates they were later changed when a PTIP for blending for rows 5 and 6 of C4 (which then randomly assigned rows 2 and 5 of C1). That is, the pairs of values having subscript a were blended yielding the blended (subscript A) values. The same is true for the subscripted b and B values.

Step 3 would now be carried out for the (C5,C2) pair producing offspring (C5*,C2*). The reproduction results of the first generation are summarized in Table 5. The elite C3 and C6 chromosomes are unchanged. Because F_D for offspring C5*, C1*, and C4* are, respectively, greater than F_D for parents C5, C1, and C4, they will replace C5, C1, and C4 in the next generation. F_D for C2*, however, is less than F_D for C2. Thus, C2 will appear again in the next generation. Because F_D is largest for C3 and C4* after the first generation, they become the elite chromosomes and C6, C2, C5*, and C1* are the parent chromosomes for the next generation.

The Step 3 process described would then be iterated (Step 4). A local grid search is then applied to the most fit chromosome (Step 5) yielding the D-optimal exact design.

6. Optimal Exact Designs

D, A, G, and IV optimal exact designs were generated for the second order model in (1) for one factor having 3 to 9 points, two factors having 6 to 12 points, and three factors having 10 to 16 points. These designs were generated using the five steps described in Section 5 where the initial population contained 16 designs. Table 1 shows that the A-optimal exact designs, the larger N designs, and 3 factor designs across all four criteria are new. Although it is not proven that these designs are exact optimal, they are the best exact designs yet to appear in the statistical literature.

Optimal Exact One Factor Designs

The optimal exact one factor designs are summarized in Table 6. For A and IV approximately 50% of the points are at or near 0. To optimize D, m points can be placed at ± 1 so that m is the smallest integer satisfying $2m > N/2$. The remaining $N - 2m$ points are set to 0. For G, when $N = 3, 6$, or 9, the points are equally distributed to ± 1 and 0. However, when $N = 4, 5, 7$ or 8, two points are chosen that are symmetric about 0. The objective function values are also given in Table 6 and can be used to calculate the relative design efficiencies defined in (2) for any other N-point design. That is, calculate the ratio of a design's $D(X)$, $A(X)$, $G(X)$ or $I(X)$ value to the italicized D^N_{opt}, A^N_{opt}, G^N_{opt}, or IV^N_{opt} value in Table 6.

Optimal Exact Two Factor Designs

The optimal exact two factor designs are summarized in Table 7. Although there are no obvious distributional patterns of points in the square, there are commonalities. For $N \geq 9$,

each design contains the four vertices $(\pm 1, \pm 1)$. Analogous to the $k = 1$ designs, more points are located near the origin $(0, 0)$ for the A and IV criteria than for the D and G criteria which have more points on the edges of the square. Like the one factor case, the objective function values in Table 8 can be used to calculate the relative design efficiencies of any other N-point design.

Optimal Exact Three Factor Designs

The optimal exact three factor designs are summarized in Table 9 and reveal some interesting patterns for the distribution of points in the cube:

- For D, the majority of points are the vertices $(\pm 1, \pm 1, \pm 1)$ (except for $N = 10$). For $N \geq 14$, the 8 vertices are included. The remaining points all lie on either the edges or faces of the cube. There are no points interior to the surface of the cube.
- For A, with $N \leq 13$, four or five vertices are included. For $N = 14, 15$, the exact designs are central composite designs (CCDs) having 0 and 1 center point, respectively. The 16 point design contains the 14-point CCD plus two replicated axial points.
- For G, symmetry is not apparent for $N = 10$ or 12. The points, however, are spread throughout the cube for these designs. For $N \geq 14$, the designs are based on the 14-point CCD. Unlike the 15-point A-optimal exact design, the replicated point is a cube vertex.
- For IV, there are obvious symmetries on subsets of cube edges and faces (except for the 14 point design). The 15 and 16 point designs are the 1 and 2 centerpoint CCDs.

The unusual coordinate choices and lack of symmetry for the 10 and 12 point G-optimal and the 14 point IV-optimal exact designs raise an important question: Are these actually optimal exact designs? Although, it is not proven that these designs are optimal exact, they are, however, the best exact designs to date. Rerunning the GA several times while varying the success probabilities for the GA probability tests did not change the results. Even if any of these designs are found not to be optimal, they will be near-optimal and be very useful for estimating relative efficiencies.

The objective function values given in Table 10 can be used to calculate the relative efficiency of any other N-point design. For example, Table 10 also contains the exact D, A, G, and IV-efficiencies of the optimal exact designs. Although these exact designs have 100% relative efficiencies for their corresponding criterion, it is interesting to see how these designs fare by the other three criteria. We see that G-efficiencies are low for the IV-optimal designs having $N \leq 14$ points and are low for the A-optimal designs having $N \leq 13$ points. Analogously, A and IV-efficiencies are low for the G-optimal designs having $N \leq 13$ points. For $N = 15, 16$, the G, A, and IV-optimal designs have efficiencies $> 90\%$ for all four criteria.

7. Relative Efficiencies of Other Three Factor Designs

The objective function values in Table 10 will be used to calculate the relative design efficiencies for the central composite designs (CCDs) of Box and Wilson [3], the small composite

designs (SCDs) of Hartley [12], the designs of Box and Draper [2], Hoke [15], and Notz [25], and designs generated by the *Optex* procedure (*SAS* Institute [26]). The relative efficiencies are presented in Tables 11 and 12. The G-efficiencies were determined by taking the maximum prediction variance on the set of 21^3 points (x_1, x_2, x_3) where $x_i \in \{\pm 1, \pm .9, \ldots 0\}$.

Because the 10-point Box-Draper design is D-optimal and has the same structure as the 10-point A and IV-optimal exact designs, its D, A and IV relative efficiencies are all $> 96\%$. The 11-point Box-Draper + 1cp design has A and IV relative efficiencies $> 98\%$ because it has the same structure as the 11-point A and IV-optimal exact designs. Both Box-Draper designs also have G-efficiencies much larger than the other 10 and 11 point designs. On a per-point basis for $N = 10, 11$, the Box-Draper design is overall the most efficient design. None of the 10 or 11 point Hoke, Notz, or SCD designs have a structure similar to any of the optimal exact designs and is reflected in their relative efficiencies.

For N=13, the Hoke D6 design has the same structure as the 13-point D-optimal exact design and is the best overall design when considering all four criteria. For $N = 14$, has the same structure as the 14-point A and G-optimal exact designs. It is also the best design by all four criteria. For $N = 15$ and 16, the CCD efficiencies at all equal to or near 100%.

Designs were also generated by the *Optex* procedure (*SAS* Institute [26]) from a set of 27 candidate points whose coordinates were ± 1 or 0. These designs, like those in Table 11, will also be irregular fractions of the 3^3 factorial design. The user has the option of several optimality criteria and several search methods for selecting design points. In this research, the Detmax and Fedorov search methods were chosen. The D and A optimality criteria options were used to search for the best exact designs that could be formed from the candidate set. Although there are no G or IV options, *SAS* will generate designs for another criterion (e.g., D or A) and then save the design having the highest G-efficiency or IV-efficiency measure. In this research, the D criterion option was selected and the designs having the best G and IV efficiencies were kept.

In *SAS*, the D and A-efficiencies are defined to be $D(X)$ and $A(X)$. The G-efficiency is defined to be $\sqrt{G(X)}$, the IV criterion is the average standard error of prediction, and both were evaluated over the 27 candidate points. For each combination of criterion, design size, and search method, the best design after forty iterations was kept. The relative efficiencies are presented in Table 12. The relative IV-efficiencies reported are based on $I(X)$ via integration (and not averaging over the candidate set). Designs generated by the *Optex* procedure will be referred to as D-best, A-best, G-best, or IV-best designs.

- The D-efficiencies for the D-best designs were very close to 100%. Their A, G and IV relative efficiencies, however, are relatively low when compared to the optimal exact designs when $N \leq 12$ but improve as N increases. Designs D10, D14f, D15, and D16 agree with the optimum designs supported by the 27 candidate points given in Atkinson and Donev [1, p.131]. Designs D14d and D14f exemplify problems associated with design-generating procedures like *Optex*. Depending on the number of iterations and the method,

designs having very different efficiencies for the other three criteria can result. Note that the A, G, and IV efficiencies are considerably lower for D14d than for D14f.

- The A-efficiencies for the A-best designs were very close to 100%. For $N \leq 13$, the G-efficiencies are poor while the D and IV efficiencies are very good. Like the 14 point D-best design, designs A14d and A14f yielded different A-best designs with the A14d design having a markedly lower G-efficiency of 48.13% compared to 100% for A14f.
- For $N \leq 13$, the G-best designs using the D-criterion do not necessarily produce designs with a high G-efficiency suggesting that the candidate set of 3^k points does not support a highly G-efficient design (which is consistent with the exact G-optimal designs in Table 9 that contain points that are not near the 27 candidate points). For $k \geq 14$, the G-best designs have high G-efficiencies. It is curious, however, that designs G15 and G16 have lower G efficiencies than designs A15 and A16. This suggests that it is not always best to use the D criterion if the goal is to generate a design with a high G efficiency. This occurs because only 3 choices for a G-best design were generated in 40 iterations.
- Recall that the IV-best design from *SAS* is based on the average standard error of prediction evaluated over the set of 27 candidate points while the IV efficiencies in Table 12 are based on the integral value $I(X)$. For $N \leq 13$, use of the D-criterion to produce IV-best designs certainly does not produce the most IV efficient designs and are particularly poor for 14 and 16 points. Note that the IV efficiencies of the A-best designs are greater than the IV efficiencies of the IV-best designs (exception for IV14d). Like the G-best designs, use of the D criterion does not necessarily generate highly IV=efficient designs because very few unique designs are generated in 40 iterations.

Although a finer grid creates a larger candidate set, *SAS* does not always yield a more G or IV-efficient design when a design is selected from a set of designs generated to optimize some other criterion, e.g. the D-criterion. For example, when using (i) the D-criterion, (ii) a candidate set of 21^3 points, and (iii) 100 design iterations, the three-factor *Proc Optex* G-best designs had $G(X) = 53.60$, 60.61, and 62.16 for $N = 10, 11, 12$, respectively, as compared to the optimal exact G^N_{opt} values of 70.27, 77.26, and 80.27. The G-best design, however, had $D(X) =$ 42.34, 44.77, and 44.39 which are very close to optimal exact D^N_{opt} values of 42.35, 44.77, and 44.99. The following warning is for experimenters who want to find an efficient design based on a particular optimality criterion: Use a design generating algorithm (such as a GA) that optimizes over the criterion of interest and not the best among those created under another criterion.

8. Conclusions

The primary goal of this research was to introduce genetic algorithms as a new and effective way to generate experimental designs and to provide a catalog of small exact response surface designs for 1, 2, and 3 factors. Tables of objective function values can be used to compare an N-point design to an exact optimal N-point design to determine relative efficiencies. This will

let the experimenter know how good a proposed design's D, A, G, and IV criterion values are relative to the best that could be expected from any implementable N-point design. Relative efficiencies for various 3 factor designs were investigated.

Although this research was limited to optimal exact response surface designs in the hypercube for second-order models, the GAs could be modified to find exact designs in spherical or irregularly-shaped design region and for other models as long as the design is not too large. Because $N \times k$ values must be found for a k factor design, it may be impractical to use a GA comparable to the one used in this research to find optimal exact designs for four or more factors and a second order model due to very large computing time requirements. For larger k, a GA, however, could be applied to several good starting designs (e.g., produced by *Optex*). This will lead to improved efficiency.

References

[1] Atkinson, A. C. and Donev, A. N. (1992). *Optimum Experimental Designs*, Oxford University Press, New York.

[2] Box, M. J. and Draper, N. R. (1974). On minimum-point second-order designs, *Technometrics*, **16**: 613-616.

[3] Box, G. E. P. and Wilson, K. B. (1951). On the experimental attainment of optimum conditions, *Journal of the Royal Statistical Society*, Ser. B, **13**, 1-45.

[4] Crary, S. B., Hoo, L., and Tennehouse, M. (1992). I-optimality algorithm and implementation, *Computational Statistics: Proceedings of the* 10^{th} *Symposium on Computational Statistics*, **2**, 209-214.

[5] Davis, L. (Ed.) (1991). *Handbook of Genetic Algorithms*, Van Nostrand Reinhold, New York.

[6] Farrell, R. H., Kiefer, J. and Walbran, A. (1967). Optimum multivariate designs, *The Proceedings of the Fifth Berkeley Symposium on Mathematical Statistics and Probability*, **1**, 113-138.

[7] Federov, V. V. (1972). *Theory of Optimal Experiments*, Academic Press, New York.

[8] Goldberg, D. E. (1989). *Genetic Algorithms in Search, Optimization, and Machine Learning*, Addison-Wesley, New York.

[9] Goldberg, D. E. (1991). Real-coded genetic algorithms, virtual alphabets, and blocking, *Complex Systems*, **5**, 139-168.

[10] Greffenstette, J. J. (Ed.) (1987). Genetic algorithms and their applications, *Proceedings of the Second International Conference on Genetic Algorithms*, Lawrence Erlbaum Assoc., Hillsdale, NJ.

[11] Haines, L. M. (1987). The application of the annealing algorithm to the construction of exact optimal designs for linear-regression models, *Technometrics*, **29**:439-447.

[12] Hartley, H. O. (1959). Smallest composite designs for quadratic response surfaces, *Biometrics*, **15**, 611-624.

[13] Hartley, H. O. and Ruud, P. G. (1969). Computer optimization of second order response surface designs, Technical Report No. 15, Texas A&M University.

[14] Haupt, R. L. and Haupt, S. E. (1998). *Practical Genetic Algorithms*, Wiley, New York.

[15] Hoke, A. T. (1974). Economical second-order designs based on irregular fractions of the 3^n factorial, *Technometrics*, **17**: 375-384.

[16] Holland, J. H. (1975). *Adaptation in Natural and Artificial Systems*, University of Michigan Press, Ann Arbor, MI.

[17] Kiefer, J. (1959). Optimum experimental designs, *Journal of the Royal Statistical Society*, Ser. B, **21**, 272-304.

[18] Kiefer, J. (1960). Optimum experimental design V, *The Proceedings of the Forth Berkeley Symposium on Mathematical Statistics and Probability*, **1**:381-405.

[19] Kiefer, J. (1961). Optimum designs in regression problems II, *Annals of Mathematical Statistics*, **32**, 298-325.

[20] Kiefer, J. and Wolfowitz, J. (1960). The equivalence of two extremum problems, *Canadian Journal of Mathematics*, **12**, 363-366.

[21] *The MathWorks*. (2000). *Matlab* High Performance Numeric Computation Software, Natick, MA.

[22] Michalewicz, Z. (1992). *Genetic Algorithms + Data Structures = Evolution Programs*, Springer-Verlag, New York.

[23] Michalewicz, Z. (Chair) (1994). *Proceedings of the First IEEE Conference on Evolutionary Computations*, **1, 2**, IEEE Service Center, Piscataway, NJ.

[24] Mitchell, T. J. (1974). An algorithm for the construction of *D*-optimal experimental designs, *Technometrics*, **16**, 203-210.

[25] Notz, W. (1982). Minimal second–order designs, *Journal of Statistical Planning and Inference*, **6**, 47–58.

[26] *SAS* Institute. (1995). *SAS/QC Software: Usage and Reference*, Version 6, First Ed., *SAS* Institute Inc., Cary, NC.

[27] Schaffer, J. D. (Ed.) (1989). *Proceedings of the Third International Conference on Genetic Algorithms*, Morgan Kaufmann Pub., San Mateo, CA.

[28] Welch, W. J. (1982). Branch-and-bound search algorithms for experimental designs based on *D*-optimality and other criteria, *Technometrics*, **24**, 41-48.

[29] Welch, W. J. (1985). ACED: algorithms for the construction of experimental designs, *American Statistician*, **39**, 146.

[30] Wynn, H. P. (1970). The sequential generation of *D*-optimum experimental designs, *Annals of Mathematical Statistics*, **41**, 1655- 1664.

Tables

Table 1 Optimal Exact Design Summary

1 Factor					2 Factors					3 Factors				
N	*D*	*A*	*G*	*IV*	*N*	*D*	*A*	*G*	*IV*	*N*	*D*	*A*	*G*	*IV*
3	A,H	*	A,H	H	6	A,B,>H,R	*	>H	>H	10	B	*	*	*
4	H	*	A,H	H	7	A,H	*	> H	>H	11	*	*	*	*
5	C,H	*	C,H	C,H	8	A,H,>R	*	>H	>H	12	*	*	*	*
6	A,>H	*	A	*	9	A,H	*	>H	>H	13	>R	*	*	*
7	*	*	*	*	10	*	*	*	*	14	*	*	*	*
8	*	*	*	*	11	*	*	*	*	15	*	*	*	*
9	A	*	A	*	12	*	*	*	*	16	*	*	*	*

References: A=Atkinson(1992), B=Box and Draper (1974), C=Crary et al (1992),
H=Haines (1987), R=Hartley and Ruud (1969)

* indicates new GA design, > indicates small improvement with the new GA design

Table 2 An Initial Population of Six Chromosomes

C1		C2		C3		C4		C5		C6	
x_1	x_2	x_1	x_2	x_1	x_2	x_1	x_2	x_1	x_2	x_1	x_2
-.9337	-.1237	-.9071	-.1487	-.5064	-.6611	-.6915	-.9618	-.3399	-.6203	-.8974	-.2314
-.4476	.1673	-.5339	.5501	-.1102	.4126	-.5580	.9207	-.7856	.2452	-.8454	.8928
.7180	-.0230	.3838	-.8247	.4964	-.3054	.9910	-.0424	.6230	-.0956	.5312	-.2679
.2019	.1090	.5051	.0111	.8950	.6654	.0993	.4589	.1682	.1201	.9461	.7488
.5551	-.7388	.1475	.4429	-.7822	.1756	.0087	.5591	.6772	-.8508	.6095	.1189
.3939	-.1762	.3633	-.6860	-.6543	.7677	.5813	.3015	-.6298	-.3679	.3794	-.1189
$F_D = 4.5466$		$F_D = 5.6010$		$F_D = 15.0231$		$F_D = 2.8114$		$F_D = 4.6747$		$F_D = 8.9734$	

Table 3 Random Deviates for Probability Tests

Blend	Zero Gene				Extreme Gene				Sign Change				Creep			
$\alpha_b = .2$	$\alpha_z = .1$				$\alpha_e = .1$				$\alpha_s = .1$				$\alpha_c = .1$			
	x_1	x_2	y_1	y_2	x_1	x_2	y_1	y_2	x_1	x_2	y_1	y_2	x_1	x_2	y_1	y_2
.79	.25	.61	.41	.30	.89	.53	.45	.34	.90	.66	.80	.27	.74	.24	.11	**.03**
.86	.64	.98	.96	.57	.91	.22	.45	.55	.61	.82	.92	.62	.90	.32	.67	.72
.42	.85	.65	.16	.84	.49	.81	.73	.83	.54	.81	.73	.30	.49	**.04**	.49	**.00**
.25	**.09**	.65	.30	.39	.59	.12	**.08**	**.06**	.18	.50	.12	.60	**.06**	.98	**.04**	.20
.03	**.03**	**.03**	.34	.14	.45	.19	.33	**.04**	.43	.39	.53	.28	.50	.14	.50	.46
.12	**.01**	.55	.78	.95	**.06**	.51	.95	.46	.17	.25	.55	.54	.13	.27	.26	.75

Table 4 First Generation Reproduction for Chromosomes C4 and C1

Initial Chromosomes			
C4		C1	
-.6915	-.9618	-.9337	-.1237
-.5580	.9207	-.4476	.1673
.9910	-.0424	.7180	-.0230
.0993	.4589	.2019	.1090
$.0087_a$	$.5591_a$	.5551	-.7388
$.5813_b$	$.3015_b$	.3939	-.1762

After blending			
C4*		C1*	
-.6915	-.9618	-.9337	-.1237
-.5580	.9207	-.4476	.2673
$.9910$	-.0424	.7180	-.0230
.0993	.4589	.2019	.1090
$-.\mathbf{2813}_A$	$.\mathbf{3101}_A$	.5551	-.7388
$.\mathbf{5644}_B$	$-.\mathbf{5390}_B$	.3939	-.1762

Zero Genes			
C4*		C1*	
-.6915	-.9618	-.9337	-.1237
-.5580	.9207	-.4476	.1673
.9910	-.0424	.7180	-.0230
0	.4589	.2019	.1090
0	**0**	.5551	.7388
0	-.5390	.3939	-.1762

Extreme Genes			
C4*		C1*	
-.6915	-.9618	-.9337	-.1237
-.5580	.9207	-.4476	.1673
.9910	-.0424	.7180	-.0230
0	.4589	**-1**	**1**
0	0	.5551	**-1**
1	-.5390	.3939	-.1762

Sign Change			
C4*		C1*	
-.6915	-.9618	-.9337	-.1237
-.5580	.9207	-.4476	.1673
.9910	-.0424	.7180	-.0230
0	.4589	-1	1
0	0	.5551	-1
1	-.5390	.3939	-.1762

ϵ values for creep ($\sigma = .2$)			
C4*		C1*	
—	—	—	−.2293
—	—	—	—
—	.2382	—	.2378
−.0075	—	.0655	—
—	—	—	—
—	—	—	—

After creeping			
C4*		C1*	
-.6915	-.9618	-.9337	**-.3530**
-.5580	.9207	$-.4476_a$	$.1673_a$
.9910	**.1958**	.7180	**.2148**
-.0075	.4589	**-.9345**	.1090
0	0	$.5551_b$	-1_b
1	-.5390	.3939	-.1762

Offspring Chromosomes			
C4*		C1*	
-.6915	-.9618	-.9337	-.3350
-.5580	.9207	-.1576	.4163
.9910	.1958	.7180	.2148
-.0075	.4589	-.9345	.1090
0	0	.5720	-.1595
1	-.5390	.3939	-.1762

Table 5 First Generation Summary

Initial Population			Offspring		Next Generation		
Chrom.	F_D	Partner	Chrom.	F_D	Chrom.	F_D	
C3	15.0321	elite	C3	15.0321	C3	15.0321	elite
C6	8.9734	elite	C6	8.9734	C6	8.9734	
C2	5.6010	C5	C2*	0.9933	C2	5.6010	
C5	4.6747	C2	C5*	10.2110	C5*	10.2110	
C1	4.5266	C4	C1*	5.6081	C1*	5.6081	
C4	2.8114	C1	C4*	13.4196	C4*	13.4196	elite

Table 6 Optimal Exact One Factor Designs and Objective Function Values

Design	Criterion	Design Points	$D(X)$	$A(X)$	$G(X)$	$I(X)$
3	D, A, G, IV	± 1, 0	*52.9134*	33.3333	100.000	0.416667
4.1	D	± 1, 0, 1	*50.0000*	27.2727	75.0000	0.340909
4.2	D, A, IV	± 1, 0^2	*50.0000*	*37.5000*	75.0000	*0.468750*
4.3	G	± 1, $\pm .4858682$	44.8422	24.8136	*82.9180*	0.369802
5.1	D	± 1, ± 1, 0	*50.3968*	24.0000	60.0000	0.300000
5.2	D	± 1, 1, 0^2	*50.3968*	34.2857	60.0000	0.428571
5.3	A	± 1, 0^3	45.7886	*36.0000*	60.0000	0.450000
5.4	G	± 1, 0, $\pm .728786$	43.8577	23.7795	*80.5763*	0.362952
5.5	IV	± 1, $.083733^2$, $-.173967$	45.6737	35.4848	60.5411	*0.450207*
6.1	D, G	± 1, ± 1, 0^2	*52.9134*	33.3333	*100.000*	0.416667
6.2	A	± 1, -1, $-.044603^3$	48.0112	*35.4332*	50.0000	0.438405
6.3	IV	± 1, -1, $-.035946^3$	48.0336	35.4280	50.0000	*0.439103*
7.1	D, A, IV	± 1, ± 1, 0^3	*51.9177*	*36.7347*	85.7143	*0.459184*
7.2	D	± 1, ± 1, 1, 0^2	*51.9177*	30.2521	85.7143	0.378151
7.3	G	± 1, ± 1, 0, $\pm .488512$	48.5210	28.6990	*91.1669*	0.393066
8.1	D	± 1, ± 1, ± 1, 0^2	*52.0021*	28.1250	75.0000	0.351563
8.2	D	± 1, ± 1, 1, 0^3	*52.0021*	34.6154	75.0000	0.432692
8.3	A, IV	± 1, ± 1, 0^4	50.0000	*37.5000*	75.0000	*0.468750*
8.4	G	± 1, ± 1, 0^2, $\pm .732051$	47.5772	27.7005	*89.1259*	0.387428
9.1	D, G	± 1, ± 1, ± 1, 0^3	*52.9134*	33.3333	*100.000*	0.416667
9.2	A, IV	± 1, ± 1, 0^5	47.8763	*37.0370*	66.6667	*0.462963*

Superscript indicates number of replicates.

Italics indicates optimal exact value D^N_{opt}, A^N_{opt}, G^N_{opt}, or IV^N_{opt}.

Table 7 Optimal Exact Two Factor Designs

Design	Crit	Design Points	a	b	c
6.1	D	$(1,1)\ (-1,1)\ (-1,-1)\ (1,-a)\ (a,-1)\ (-b,b)$	.394449	.131483	
6.2	A	$(1,-1)\ (-1,-1)\ (0,1)\ (-1,a)\ (1,a)\ (0,b)$	.503816	$-.220484$	
6.3	G	$(-1,-1)\ (a,a)\ (1,b)\ (b,1)\ (c,-1)\ (-1,c)$	$-.193256$	.522	.864001
6.4	IV	$(-1,1)\ (a,1)\ (-1,-a)\ (1,-b)\ (b,-1)\ (-c,c)$	.707479	.276367	.144868
7.1	D	$(\pm1,\pm1)\ (1,-a)\ (a,-1)\ (-b,b)$	.067476	.091516	
7.2	A	$(-1,-1)\ (1,-1)\ (0,1)\ (-1,a)\ (1,a)\ (0,b)^2$	.478014	$-.218806$	
7.3	G	$(1,1)\ (a,-1)\ (-1,a)\ (b,-1)\ (-1,b)\ (c,d)\ (d,c)$	.937817	$-.603132$	.773037
				$d=-.050674$	
7.4	IV	$(1,-1)\ (-1,a)\ (-a,1)\ (1,b)\ (-b,-1)\ (c,-c)^2$	.310497	.796856	.147869
8.1	D	$(\pm1,\pm1)\ (0,1)\ (\pm1,a)\ (0,b)$	.082078	$-.215160$	
8.2	A	$(-1,-1)\ (-1,1)\ (1,-1)\ (a,1)\ (1,b)\ (c,d)^2\ (-1,e)$	.078929	.571386	$-.029071$
				(d,e)=(–.179098,.100290)	
8.3	G	$(\pm1,\pm1)\ (1,-a)\ (-1,a)\ (-b,-c)\ (b,c)$	.052190	.063291	.824605
8.4	IV	$(1,-1)\ (-1,1)\ (-1,-a)\ (a,1)\ (1,b)\ (-b,-1)\ (c,-c)^2$	.003859	.768301	.094936
9.1	D,A	$(\pm1,\pm1)\ (0,\pm1)\ (\pm1,0)\ (0,0)$			
9.2	G	$(\pm1,\pm1)\ (0,0)\ (a,1)\ (-a,-1)\ (1,-a)\ (-1,a)$	.420229		
9.3	IV	$(-1,1)\ (-1,-1)\ (-1,0)\ (a,1)\ (a,-1)\ (1,b)\ (1,-b)\ (c,0)^2$	.044158	.836727	.044687
10.1	D	$(\pm1,\pm1)\ (1,-1)\ (1,a)\ (-a,-1)\ (-b,1)\ (-1,b)\ (c,-c)$	.099329	.016983	.024346
10.2	A,IV	$(\pm1,\pm1)\ (0,\pm1)\ (\pm1,0)\ (0,0)^2$			
10.3	G	$(\pm1,\pm1)\ (0,-1)\ (\pm1,a)\ (\pm b,1)\ (0,c)$	$-.430$	.564028	.176604
11.1	D	$(\pm1,\pm1)\ (-1,-1)\ (1,-1)\ (0,\pm1)\ (\pm1,a)\ (0,b)$	.107871	$-.047248$	
11.2	A,IV	$(\pm1,\pm1)\ (0,\pm1)\ (\pm1,0)\ (0,0)^3$			
11.3	G	$(\pm1,\pm-1)\ (-1,-1)\ (1,a)\ (a,1)\ (b,-1)\ (-1,b)$	$-.561111$	.158889	.819313
		$(c,c)\ (d,d)$		$d=.000843$	
12.1	D	$(\pm1,\pm1)\ (-1,-1)\ (1,\pm1)\ (1,a)\ (-a,-1)\ (-1,b)\ (-b,1)$	.006125	.101286	.023820
		$(c,-c)$			
12.2	A	$(\pm1,\pm1)\ (1,0)^2(-1,0)\ (a,-1)\ (a,1)\ (b,0)^3$	.059358	$-.021281$	
12.3	G	$(1,-1)\ (-1,1)\ (1,a)\ (a,1)\ (b,-1)\ (-1,b)\ (c,d)\ (d,c)$	$-.681289$	.061178	.519483
		$(1,e)\ (e,1)\ (-1,-e)\ (-e,-1)$		(d,e)=(–.035116,.895400)	
12.4	IV	$(\pm1,\pm1)\ (0,\pm1)\ (\pm1,0)\ (0,0)^4$			

Superscript indicates number of replicates.

Table 8 Objective Function Values for Optimal Exact Two Factor Designs

Design	Crit	$D(X)$	$A(X)$	$G(X)$	$I(X)$
6.1	D	*42.3123*	23.7678	53.6542	0.203900
6.2	A	40.2493	*24.9498*	47.6404	0.215497
6.3	G	40.0282	22.4212	*74.7848*	0.201153
6.4	IV	38.5778	24.2674	43.3045	*0.217679*
7.1	D	*45.0294*	26.5980	62.7317	0.216525
7.2	A	38.5353	*27.7966*	43.4494	0.246567
7.3	G	39.6551	21.2708	*80.1917*	0.187068
7.4	IV	38.3264	27.4265	45.1872	*0.249073*
8.1	D	*45.6158*	28.8985	66.5008	0.226189
8.2	A	41.6175	*29.3007*	46.5486	0.252940
8.3	G	44.4993	26.0074	*87.9430*	0.207269
8.4	IV	40.9190	28.9988	57.1103	*0.255705*
9.1	D,A	*46.2241*	*31.1688*	82.7586	0.246914
9.2	G	43.3872	25.1256	*86.3495*	0.211777
9.3	IV	41.9300	30.5841	60.8100	*0.260546*
10.1	D	*45.9888*	29.3382	75.9635	0.230390
10.2	A,IV	44.7808	*33.3775*	75.2239	*0.273319*
10.3	G	43.3727	25.2835	*85.9373*	0.206222
11.1	D	*46.1515*	28.1127	70.8426	0.217902
11.2	A,IV	42.8354	*33.3415*	68.7092	*0.278842*
11.3	G	43.3501	24.0550	*86.2093*	0.197660
12.1	D	*46.6212*	27.1382	66.4776	0.208571
12.2	A	42.0773	*32.7815*	62.3629	0.272210
12.3	G	41.5950	23.6147	*84.8966*	0.203403
12.4	IV	40.8248	32.4324	63.1579	*0.275229*

Italics indicates optimal exact value D^N_{opt}, A^N_{opt}, G^N_{opt}, or IV^N_{opt}.

Table 9 Optimal Exact Three Factor Designs

	D-optimal			A-optimal			G-optimal			IV-optimal		
	x_1	x_2	x_3	x_1	x_2	x_3	x_1	x_2	x_3	x_1	x_2	x_3
	.2912	-1	-1	-.1749	-1	1	-.9998	.4518	.8786	-.9605	-.1025	-.1025
	-1	.2912	-1	1	.1749	1	1	1	.3059	.1025	.9605	-.1025
	-1	-1	.2912	1	-1	-.1749	1	-1	-.9110	.1025	-.1025	.9605
$n=10$	-.1925	1	-.1925	-1	-.1072	.1072	-.8810	-1	.9900	-.2553	-1	-1
	-.1925	-.1925	1	.1072	1	.1072	-1	-.7809	-1	1	.2553	-1
	1	-.1925	-.1925	.1072	-.1072	-1	.0615	1	1	1	-1	.2553
	-1	1	1	-1	1	-1	1	-.6490	1	-1	1	1
	1	1	-1	-1	1	1	-.9558	1	-.7944	1	1	1
	1	-1	1	1	1	-1	.7592	.6918	-1	-1	1	-1
	1	1	1	-1	-1	-1	-.0413	-.5508	-.0283	-1	-1	1

	x_1	x_2	x_3	x_1	x_2	x_3	x_1	x_2	x_3	x_1	x_2	x_3
	1	0	0	.1223	-1	1	-.1140	-1	1	-.0589	.0589	-.0589
	0	1	0	-1	.1223	1	-1	-.1140	1	-1	-.1905	.1905
	0	0	1	-1	-1	-.1223	-1	-1	.1140	.1905	1	.1905
	±1	±1	±1	-.2166	-.2166	-1	-.7550	-.7550	-1	.1905	-.1905	-1
$n=11$				-.2166	1	.2166	-.7550	1	.7550	-.2349	-1	1
				1	-.2166	.2166	1	-.7550	.7550	1	.2349	1
				.0914	.0914	-.0914	.1858	.1858	-.1858	1	-1	-.2349
				1	-1	-1	1	-1	-1	-1	-1	-1
				1	1	-1	1	1	-1	-1	1	-1
				-1	1	-1	-1	1	-1	-1	1	1
				1	1	1	1	1	1	1	1	-1

	x_1	x_2	x_3	x_1	x_2	x_3	x_1	x_2	x_3	x_1	x_2	x_3
	1	-.0150	-.0150	.1185	1	1	1	-.7188	1	-.0925	-.0925	.0925
	-.0150	1	-.0150	-1	-.1185	1	1	-1	-.9960	-.0925	-.0925	.0925
	-.0150	-.0150	1	-1	1	.0814	-1	-1	-.9900	-1	.3120	-.3120
	.0426	-1	-1	.0232	-.0232	-.1403	.9930	.9841	.8816	.3120	-1	-.3120
	±1	±1	±1	-.1811	-1	.2417	-1	1	-.8898	.3120	.3120	1
$n=12$				1	.1811	.2417	-1	-.5815	1	-.1685	1	-1
				-.0474	.0474	-1	-.4144	-1	.9600	1	-.1685	-1
				-1	1	-1	-.7357	1	.9983	1	1	.1685
				-1	-1	-1	.9998	1	-.8238	-1	-1	1
				1	1	-1	-1	.0100	.0940	1	-1	1
				1	-1	-1	.3524	-1	.0469	-1	-1	-1
				1	-1	1	.0928	.0913	-1	-1	1	1

Table 9 Optimal Exact Three Factor Designs (continued)

	D-optimal			*A*-optimal			*G*-optimal			*IV*-optimal		
	.1463	1	1	0	-.0537	0	.3938	-1	-1	0	-.0537	0
	1	.1463	1	0	-.0537	0	1	-.3938	-1	0	-.0537	0
	1	1	.1463	-.1243	1	1	1	-1	-.3938	-.1243	1	1
	.0644	.0644	-1	.1243	1	-1	-1	0	0	.1243	1	-1
	.0644	-1	.0644	1	-.6353	-1	0	1	0	1	-.6353	-1
	-1	.0644	.0644	-1	-.6353	1	0	0	1	-1	-.6353	1
$n = 13$	-1	-1	1	1	.2472	1	1	-1	1	1	.2472	1
	-1	1	-1	-1	.2472	-1	1	1	-1	-1	.2472	-1
	1	-1	1	1	1	-.1243	1	1	1	1	1	-.1243
	-1	-1	-1	-1	1	.1243	-1	-1	-1	-1	1	.1243
	1	-1	-1	0	-1	0	-1	-1	1	0	-1	0
	-1	1	1	-1	-1	-1	-1	1	-1	-1	-1	-1
	1	1	-1	1	-1	1	-1	1	1	1	-1	1

	x_1	x_2	x_3	x_1	x_2	x_3	x_1	x_2	x_3	x_1	x_2	x_3
	-.0187	1	1	-1	0	0	-1	0	0	-.8052	1	1
	1	-.0187	1	1	0	0	1	0	0	-.5653	-1	-1
	1	1	-.0187	0	-1	0	0	-1	0	-1	-.1528	1
	.0583	.0583	-1	0	1	0	0	1	0	-1	-1	.0475
	.0583	-1	.0583	0	0	-1	0	0	-1	.3061	-1	1
	-1	.0583	.0583	0	0	1	0	0	1	1	-1	-.7339
$n = 14$	±1	±1	±1	±1	±1	±1	±1	±1	±1	1	.8613	1
										-1	.9168	-1
										1	1	-1
										1	-.1531	.1993
										-.0174	1	.0152
										.0524	-.0482	-1
										-.0240	.0628	-.0056
										-.0240	.0628	-.0056

	-.0760	-1	1	-1	0	0	-1	0	0	-1	0	0
	-.0273	-1	-1	1	0	0	1	0	0	1	0	0
	-1	-.0905	-.0282	0	-1	0	0	-1	0	0	-1	0
$n = 15$	1	.0305	-1	0	1	0	0	1	0	0	1	0
	1	-1	.0193	0	0	-1	0	0	-1	0	0	-1
	.0730	1	-.0417	0	0	-1	0	0	-1	0	0	-1
	.1205	.0431	1	0	0	0	1	-1	-1	0	0	0
	±1	±1	±1	±1	±1	±1	±1	±1	±1	±1	±1	±1

Table 9 Optimal Exact Three Factor Designs (continued)

	D-optimal			*A*-optimal			*G*-optimal			*IV*-optimal		
	.0513	1	-1	-1	0	0	-1	0	0	-1	0	0
	1	1	-.0513	1	0	0	1	0	0	1	0	0
	.0290	1	1	0	-1	0	0	-1	0	0	-1	0
	-1	1	-.0290	0	1	0	0	1	0	0	1	0
$n = 16$	-.0819	-.0258	-1	0	0	-1	0	0	-1	0	0	-1
	1	-.0258	-1	0	0	-1	0	0	-1	0	0	-1
	1	-.0258	.0819	0	-1	0	0	1	0	0	0	0
	-1	-.0426	1	1	0	0	1	0	0	0	0	0
	±1	±1	±1	±1	±1	±1	±1	±1	±1	±1	±1	±1

Table 10 Properties of Optimal Exact Three Factor Designs

		Objective Function Values				Relative Efficiencies			
Design	Crit	$D(X)$	$A(X)$	$G(X)$	$I(X)$	D^N_{eff}	A^N_{eff}	G^N_{eff}	IV^N_{eff}
10.1	D	*42.3472*	26.2481	54.3289	0.141268	100	97.67	77.32	96.85
10.2	A	41.9959	*26.8743*	46.4859	0.144570	99.17	100	66.16	99.11
10.3	G	38.7061	20.1709	*70.2670*	0.115335	91.40	75.06	100	79.07
10.4	IV	41.3179	26.1979	48.6854	*0.145864*	97.57	97.48	69.29	100
11.1	D	*44.7689*	21.3904	60.6061	0.117302	100	74.04	78.44	70.97
11.2	A	40.8874	*28.8912*	45.1013	0.164403	91.33	100	58.37	99.47
11.3	G	41.7556	22.5289	*77.2634*	0.123903	93.27	77.98	100	74.97
11.4	IV	40.9691	28.7335	49.1957	*0.165276*	91.51	99.45	63.67	100
12.1	D	*44.9860*	22.3639	55.6322	0.119782	100	77.36	69.31	70.39
12.2	A	42.1774	*28.9086*	42.2589	0.163832	93.76	100	52.65	96.27
12.3	G	41.8562	22.3760	*80.2657*	0.118096	93.04	74.40	100	69.40
12.4	IV	39.4351	28.6228	48.0329	*0.170177*	87.66	99.01	59.84	100
13.1	D	*46.3911*	26.9475	80.1026	0.137513	100	90.87	95.66	80.50
13.2	A, IV	40.2720	*29.6687*	54.5010	*0.170833*	86.81	100	65.08	100
13.3	G	45.6993	25.4346	*83.7388*	0.130210	98.51	85.76	100	76.22
14.1	D	*46.3262*	26.3491	83.2924	0.134015	100	84.84	93.29	76.78
14.2	A, G	46.3045	*31.0559*	*89.2857*	0.171429	99.95	100	100	98.22
14.3	IV	39.8889	29.6854	47.3980	*0.174538*	86.10	95.59	53.09	100
15.1	D	*46.0281*	26.2457	78.1792	0.131732	100	83.88	93.16	72.64
15.2	A, IV	44.7163	*31.2907*	83.6237	*0.181360*	97.15	100	99.65	100
15.3	G	45.8339	29.6479	*83.9161*	0.163543	99.58	94.75	100	90.18
16.1	D	*45.8851*	26.4025	73.7878	0.130717	100	83.43	92.97	71.22
16.2	A, G	44.5097	*31.6456*	79.3651	*0.175097*	97.00	100	100	95.40
16.3	IV	42.9990	30.6813	78.5482	*0.183544*	93.71	96.95	98.97	100

Italics indicates optimal exact value D^N_{opt}, A^N_{opt}, G^N_{opt}, or IV^N_{opt}.

Table 11 Relative Efficiencies for Various Three Factor Designs

N	Design	D_{eff}^N	A_{eff}^N	G_{eff}^N	IV_{eff}^N
10	Box-Draper	100	97.67	77.32	96.85
	Hoke D1, Notz	94.46	63.34	20.33	62.32
	Hoke D2	94.46	72.61	20.33	64.27
	Hoke D3	85.98	58.14	11.15	62.10
	SCD	71.59	67.66	20.33	66.35
11	Box-Draper+cp	91.54	98.62	65.68	99.73
	Hoke D1+cp, Notz+cp	88.56	70.28	22.13	74.67
	Hoke D2+cp	87.06	71.48	18.10	69.00
	Hoke D3+cp	79.24	56.19	9.46	61.39
	SCD+cp	63.83	59.44	16.83	55.94
13	Hoke D4	91.51	93.86	22.97	90.43
	Hoke D5	88.60	68.33	15.68	62.60
	Hoke D6	99.35	90.45	77.73	80.66
	Hoke D7	82.05	61.01	8.62	66.64
14	CCD (0 cp)	99.95	100	100	98.22
	Hoke D4+cp	88.17	89.67	20.35	91.50
	Hoke D5+cp	87.98	76.43	16.00	76.64
	Hoke D6+cp	97.54	94.88	70.26	94.71
	Hoke D7+cp	80.24	64.01	8.89	72.59
15	CCD (1 cp)	97.15	100	99.65	100
16	CCD (2 cp)	93.71	96.95	98.97	100

Table 12 Relative Efficiencies for *Proc Optex* Three Factor Designs

N	Crit.	Method	Design	D_{eff}^N	A_{eff}^N	G_{eff}^N	IV_{eff}^N
10	D	both	D10	96.71	81.19	41.32	79.79
	A	both	A10	95.47	95.90	49.19	93.54
	G	detmax	G10d	94.46	52.92	48.65	42.26
	G	fedorov	G10f	91.30	85.87	57.35	86.72
	IV	detmax	IV10d	96.71	81.19	41.32	79.79
	IV	fedorov	IV10f	91.30	85.87	57.35	86.72
11	D	both	D11	100	74.04	78.44	70.97
	A	both	A11	86.87	93.02	40.91	91.02
	G	both	G11	100	74.04	78.44	70.97
	IV	detmax	IV11d	100	74.04	78.44	70.97
	IV	fedorov	IV11f	93.01	88.55	62.58	80.14
12	D	both	D12	99.98	77.32	69.50	70.27
	A	both	A12	90.74	95.34	38.24	90.95
	G	both	G12	99.98	77.32	69.50	70.27
	IV	detmax	IV12d	94.19	94.58	58.83	83.73
	IV	fedorov	IV12f	99.98	77.32	69.50	70.27
13	D	both	D13	99.35	90.45	77.73	80.66
	A	both	A13	88.69	98.30	52.35	94.05
	G	both	G13	99.35	90.45	77.73	80.66
	IV	both	IV13	99.35	90.45	77.73	80.66
14	D	detmax	D14d	99.88	84.60	92.90	76.48
	D	fedorov	D14f	99.95	100	100	98.22
	A	detmax	A14d	87.89	96.21	48.13	95.99
	A	fedorov	A14f	99.95	100	100	98.22
	G	detmax	G14d	99.88	84.60	92.90	76.48
	G	fedorov	G14f	99.95	100	100	98.22
	IV	detmax	IV14d	99.95	100	100	98.22
	IV	fedorov	IV14f	99.88	84.60	92.90	76.48
15	D	both	D15	99.83	83.70	92.41	72.45
	A	both	A15	97.15	100	99.65	100
	G	both	G15	99.83	83.70	92.41	72.45
	IV	detmax	IV15d	99.83	83.70	92.41	72.45
	IV	fedorov	IV15f	99.58	94.75	100	90.18
16	D	both	D16	99.89	83.28	93.45	70.95
	A	both	A16	97.00	100	100	95.40
	G	detmax	G15d	99.89	83.28	93.45	70.95
	G	fedorov	G15f	99.28	89.87	99.91	85.38
	IV	both	IV16	99.89	83.28	93.45	70.95