

OPTIMAL EXPERIMENTAL DESIGNS IN TWO DIMENSIONS
USING MINIMUM BIAS ESTIMATION

J. W. Evans and A. R. Manson

Institute of Statistics
Mimeograph Series No. 939
Raleigh

OPTIMAL EXPERIMENTAL DESIGNS IN TWO DIMENSIONS USING
MINIMUM BIAS ESTIMATION

J. W. EVANS and A. R. MANSON^{*}

ABSTRACT

The general problem of minimum bias estimation is reviewed for polynomial response surface models, where the true model, a polynomial of degree $d+k-1$, is estimated by a polynomial of degree $d-1$. Through the choice of estimator, the same minimum integrated squared bias B is achieved for any experimental design that satisfies a simple estimability condition. This design flexibility is used to construct D-optimal, V-optimal, and A-optimal experimental designs in two dimensions through a computerized simplex search procedure. The resulting optimal designs for both square and circular regions of interest are discussed and recommendations as to their use are made.

* J. W. Evans is a graduate student and A. R. Manson is an Associate Professor, Department of Statistics, North Carolina State University, Raleigh, N.C. 27607

1. INTRODUCTION

The study of design optimality criteria has always been of fundamental importance in response surface analysis, especially when the functional form of the response surface relationship

$$\eta = f(\tau_1, \dots, \tau_p; \theta_1, \dots, \theta_r) = f(\underline{\tau}, \underline{\theta}), \quad (1.1)$$

is unknown. It is common practice to approximate the functional relationship $f(\underline{\tau}, \underline{\theta})$ by a polynomial of degree m , denoted P_m , and then fit the standard polynomial model using least squares methods. Various properties of the resulting fitted polynomials have been investigated, especially those properties which are heavily influenced by the choice of the experimental design.

Most major design criteria such as D-optimality, G-optimality, rotatability, etc., have one thing in common. They are "variance criteria" which assume that the model to be fitted is the true model. The question of bias due to the inadequacy of the approximating polynomial is often given little consideration. This can be a serious oversight as has been pointed out by several authors [1, 2, 4, 10, 13]. For example, D-optimal and G-optimal designs are extremely model dependent. It is important therefore to look at design criteria that take into account the concept of bias as well as variance.

2. MINIMUM BIAS ESTIMATION

Suppose the true model is a polynomial of degree $d+k-1$

$$\eta(\underline{x}) = \underline{x}'\underline{\beta}_1 + \underline{x}'\underline{\beta}_2 \quad (2.1)$$

but for one reason or another is estimated by a polynomial of degree $d-1$

$$\hat{\eta}(\underline{x}) = \underline{x}'\underline{b}_1 \quad (2.2)$$

Discrepancies between the true response and fitted model stem from both variance (i.e., sampling error) and bias (inadequacy of the approximating polynomial).

Box and Draper in 1959 [1] and again in 1963 [2] adopted the minimization of mean square error integrated over a region of interest R (denoted IMSE) as a basic criterion. This criterion involves both variance and bias. The IMSE for R, the region of experimental interest, is

$$J = \frac{N\Omega}{2} \int_R E\{\hat{y}(\underline{x}) - \eta(\underline{x})\}^2 d\underline{x} \quad (2.3)$$

where

$$\Omega^{-1} = \int_R d\underline{x} . \quad (2.4)$$

It is easy to show that J is the sum of integrated squared bias,

$$B = \frac{N\Omega}{2} \int_R \{E[\hat{y}(\underline{x})] - \eta(\underline{x})\}^2 d\underline{x} . \quad (2.5)$$

and integrated Var $\hat{y}(\underline{x})$,

$$V = \frac{N\Omega}{2} \int_R \text{Var } \hat{y}(\underline{x}) d\underline{x} . \quad (2.6)$$

Minimization of $J = V+B$ requires advance knowledge of the regression coefficients. Such prior knowledge is generally not available. Box and Draper attacked this lack of prior knowledge by minimizing the average value of J over all orthogonal rotations of the response surface. In the process, they showed that unless V is at least four times B, optimal designs for minimizing the sum of V and B have design moments which are close to those obtained by assuming $V = 0$.

Box and Draper proposed that an experimenter (1) estimate $\underline{\beta}_1$ using standard least squares, and (2) find an experimental design which minimizes B. The design, which minimizes B for the standard least squares estimator, is one which satisfies

$$(X_1 X_1)^{-1} X_1 X_2 = W_{11}^{-1} W_{12} \quad (2.7)$$

where

$$W_{ij} = \Omega^{-1} \int_R \underline{x}_i \underline{x}_j' d\underline{x} . \quad (2.8)$$

W_{ij} is a moment matrix of a uniform probability distribution over the region

of interest R . Designs which satisfy (2.7) are said to meet the Box and Draper condition.

In 1969, Karson, Mansou, and Hader [10] minimized B through the choice of the estimator. If \underline{b}_1 is to minimize the bias term B , $E(\underline{b}_1)$ must satisfy

$$E(\underline{b}_1) = A\beta \quad (2.9)$$

where

$$A = [1:W_{11}^{-1}:W_{12}] \quad (2.10)$$

and

$$\beta' = (\beta_1':\beta_2') \quad (2.11)$$

The minimized value of B is easily shown to be

$$\text{Min } B = \frac{N\Omega}{2} \beta_2' \{W_{22} - W_{12}' W_{11}^{-1} W_{12}\} \beta_2 \quad (2.12)$$

where W_{ij} is given in (2.8). The exact same Min B value is achieved for any design for which $A\beta$ is estimable.

Karson, Manson and Hader go on to show in their paper that the estimator $\underline{b}_1 = T'y$, called the "minimum bias estimator" (MBE), where

$$T' = AGX' \quad (2.13)$$

and where G is the generalized inverse of $X'X$, minimizes the integrated variance V subject to minimum B for any fixed design. Note that $X = (X_1':X_2')$. V was then further minimized by choice of the experimental design. In this manner Karson, Manson, and Hader were able to achieve smaller IMSE than by using the Box and Draper approach.

3. DESIGN OPTIMALITY CRITERIA

Thus, by choice of the estimator, minimized integrated squared bias B , due to terms of specified higher degree from the fitted response, is achieved for any design for which $A\beta$ is estimable. From this large class of designs, designs can be found that are D-optimal, V-optimal or A-optimal.

A design is said to be D-optimal for the model $\hat{y}(\underline{x})$ given in (2.2), if it minimizes the determinant of the variance covariance matrix of $\hat{\underline{b}}_1$. Using minimum bias estimation, this means that a design is D-optimal if it minimizes $|(AGA')|$ or equivalently if it maximizes $|(AGA')^{-1}|$. Another popular design criterion is G-optimality. A design is said to be G-optimal for the model $\hat{y}(\underline{x})$ if it minimizes $\max_{\underline{x}_u} \text{var}(\hat{y}_u)$ where $\hat{y}_u = \underline{x}_u' \hat{\underline{b}}_1$. As is the case when using standard least squares, a design is D-optimal using the MBE if and only if it is G-optimal for the MBE. The variance criterion of D-optimality (and equivalently G-optimality) shall be denoted by V_1 .

Using D and G optimality criteria for designing experiments produces designs which for the MBE

1. Have a confidence region for the parameters of smallest (hyper) volume in the parameter space,
2. Minimize the generalized variance of the minimum bias parameter estimates,
3. Are invariant to linear changes of scale of the parameters,
4. Minimize the maximum variance of any predicted value (from the regression function) over the experimental space.

Minimizing the integrated variance, V , used by Box and Draper and Karson, Manson and Hader produces designs that are V-optimal, a design criterion that shall be denoted by V_2 . For the MBE, V-optimal designs are obtained by minimizing $N \text{ trace}(AGA'W_{11})$. The use of the MBE and V-optimal designs achieves the same minimum IMSE found by Karson, Manson, and Hader.

A design is said to be A-optimal for the model $\hat{y}(\underline{x})$ in (2.2), if it minimizes the trace of the variance covariance matrix of $\hat{\underline{b}}_1$. Thus the variance criterion V_2 shall denote the A-optimal design criterion when the MBE is used. For the MBE, A-optimal designs minimize the trace (AGA') . This minimizes the

average variance of the parameter estimates. V_3 is not invariant to linear changes of scale of the parameters as are V_1 and V_2 .

The advantages and disadvantages of each of these three variance criteria have been discussed numerous times in the literature. It is not the purpose of this paper to repeat the well-known arguments for each criterion. Instead, using the MBE, optimal designs for each criterion are developed and are used to compare the criteria.

4. DESIGNS

A computer program was written to aid in the searching for optimal designs for which AB is estimable. This program employs the simplex search procedure suggested by Hendrix [9]. As a check on the effectiveness of the simplex search procedure used, the computer program was applied to the problems of finding D-optimal designs for situations studied by Dykstra [5] and by Mitchell [11,12]. In no situation did the simplex search procedure fail to match the published results. It is the results of this program's search that are being presented here.

Extensive use of the program repeatedly demonstrated that the optimal designs for each variance criterion are basically concentric n-gons. Thus designs will be denoted as combinations of regular n-gons which are concentric about the origin. Each n-gon is described by the notation (N,θ) where N is the number of vertices and θ is the counterclockwise rotation of a reference vertex from the positive x_1 -axis. In two dimensions ($q=2$), which is the situation dealt with in this paper, there is no reason for loss of generality with this notation. Any design can be represented in this manner since each n-gon could contain only one point. The radius of the i^{th} n-gon in a design will be specified by the parameter ρ_i , while the number of observations taken at the origin will be denoted by N_0 .

4.1 Designs for Linear Polynomials Protecting Against Quadratic Effects

Suppose that in two dimensions ($q=2$) the true model is quadratic ($d+k-1=2$) but is fitted by a linear model ($d-1=1$). This design setting will be denoted as

$$(q=2, d=2, k=1) .$$

For this setting, designs have been studied for $3 \leq N \leq 9$. For $N=3$ and $N=4$ there are no designs for which $A\beta$ is estimable. For $5 \leq N \leq 9$ designs for which $A\beta$ is estimable were thoroughly searched.

Tables 1, 2, and 3 give the best designs found for each of the three variance criteria for a square region of interest, (SRI). The choice of a square (or rectangular) region of interest by an experimenter is a natural choice. Most experimenters have a range of interest for each of k variables, that is to say they are interested in the i^{th} variable between the values a_i and b_i for $i = 1, 2, \dots, k$. This interest is quite naturally satisfied by a square (or rectangular) region of interest.

A brief comparison of the designs in Tables 1, 2, and 3 shows a number of general characteristics of the three variance criteria. The most important characteristic is that every optimal design found for a square region of interest contains at least one observation in the corners of the region of interest. If the experimenter has a SRI, it is necessary to place at least one observation in each corner if an optimal or near optimal design for any of the three variance criteria is desired.

For the SRI, the same optimal design was found for all three criteria when $N=5$ and when $N=6$. This is the result of the restriction that $A\beta$ be estimable and the importance of the shape of the region of interest. Not until designs have seven or more points does the restriction of $A\beta$ being

estimable cease to produce the same optimal design for each variance criterion for a SRI.

Table 1 contains the optimal designs found for V_1 for a SRI. These optimal designs for V_1 , with the exception of $N=7$, are all singular designs. Thus an experimenter could not change his mind after experimentation and fit a quadratic model if he so desired. Also V_1 suffers from the disadvantage of possessing many local optima. For both $N=8$ and $N=9$, the best design found was unapproachable by a search routine because of singularity problems. The criterion of D-optimality often has the problem of search routines stopping at local optima [8]. Therefore several designs that were singular with respect to the true model, but for which $\underline{A\hat{\theta}}$ is estimable, were searched. This resulted in the discovery of the designs for $N=8$ and $N=9$ listed in Table 1. The real nature of the problem of locating optima in such situations using direct search computer routines, appears to be the occasional lack of continuity between singular and non-singular designs.

The optimal design for $N=8$ for V_1 in a SRI is somewhat inefficient for V_2 and V_3 . A better design for all three criteria is

	$\frac{N_0}{\rho_0}$	$\frac{\rho_1}{\rho_0}$	$\frac{\rho_0}{\rho_1}$	$\frac{V_1}{\rho_0}$	$\frac{V_2}{\rho_0}$	$\frac{V_3}{\rho_0}$
$(4, \frac{\pi}{4}) + (4, 0)$	0	2	.582	128.1	2.51	.598

Unless the experimenter knows that he is definitely interested in a D-optimal experimental design, he might want to use a design that is near optimal for all three criteria. The design above is V_1 optimal for two 4-gons and also has values of V_2 and V_3 which are very close to their optimal values.

It is important to be able to compare the "size" of different designs. The comparisons that we will make among the three variance criteria will depend to some extent on how we define "size". We shall adopt the definition of "size" proposed by Box and Wilson [3]. If a design consists of K factors

and N observations, S_t is called the spread for the t^{th} variable where

$$S_t = \frac{\sum_{u=1}^n (x_{tu} - \bar{x}_t)^2}{N} . \quad (4.1.2)$$

Two designs are considered to be of comparable size if the spread of each of the factors is the same in the two designs. When designs are not of comparable size, total spread, denoted by

$$TS = \sum_{t=1}^k S_t \quad (4.1.3)$$

will be used to compare designs. Furthermore, variance criterion V_i will be said to be more highly "variance oriented" than variance criterion V_j if the optimal designs found for V_i have a total spread greater than the optimal designs of the same size found for V_j .

On the basis of these definitions, a comparison of the three variance criteria is possible. Tables 4, 5, and 6 give the best designs found for each of the three variance criteria for a circular region of interest, (CRI). These tables of optimal designs for the CRI show clearly that V_3 produces designs with the greatest total spread and V_2 produces designs with the least total spread. For a CRI, a high total spread generally means that most of the observations will be on the boundary of the region of interest. Of the resulting fifteen optimal designs found, only two designs had observations located at points other than at the center of or on the boundary of the region of interest. Consequently, the size of the region of interest and the number of points on the boundary are of critical importance if a CRI is used.

For the SRI such complete ordering is not possible. This is because some of the optimal designs found for V_1 are singular and unapproachable by a search routine. If we ignore these unusual situations and compare the variance criteria for a SRI for nonsingular designs of the same configuration of n -gons,

the relationship of V_3 being the most highly variance oriented criterion and V_2 being the least, holds true.

All things considered, V_2 is recommended as a primary variance criterion. There are several reasons for this preference. With the exception of only one design, all of the optimal designs found for V_1 for both a square and a circular region of interest consist of only boundary points and center points. Designs of this type are of questionable value for two reasons:

1. Extensive regions of the response surface remain unobserved.
2. Fitted polynomials based on such designs are not always good for prediction purposes in the interior of the region of interest. The variance of predicted values is related to the uniform information over the whole region of interest. Designs consisting only of boundary and center points produce little information anywhere else and hence produce high variance of predicted values anywhere except near the boundary and near the center of the region of interest.

The optimal V_1 designs found for a SRI for $N=8$ and $N=9$ are of a special nature due to their unapproachability by a search routine. In these designs, two diagonal corner points of the region of interest are replicated, along with 2 or 3 center points. If observations are taken near the center of the region of interest but not exactly at the center, the resulting design has a value of V_1 less than one half the optimal value of V_1 . To have such a small change in location of points make such a large difference in the value of V_1 is not a pleasing result. Since neither V_2 nor V_3 seems so affected by local optima and since both do produce designs with more information about the interior of the region of interest than does V_1 , they are both preferred to V_1 .

The choice of V_2 over V_3 is based on a number of pleasing characteristics that V_2 contains that V_3 does not. V_2 is the only variance criterion scaled to take into account differences in the number of points between two designs and different areas for regions of interest. The result of such scaling is a measurement of variance per observation per unit area. This makes it feasible to compare designs of different sizes and in a limited sense from different regions of interest. Neither V_1 nor V_3 are averaged over the region of interest. Consequently they are not scaled as meaningfully as is V_2 . Thus it is felt a more accurate idea about the relative efficiency of a given design is obtained by using V_2 than by using V_3 .

V_2 is also preferred over V_3 because it is less highly variance oriented. It often seems simpler to define a region of operability than a region of interest. Therefore the region of operability is often used as the region of interest simply because of the difficulty of deciding just what region inside of the operability region is really the region of interest. When one chooses the region of interest in this way, V_2 will produce designs with more information about the interior of the region of operability, and hence about the true region of interest, than will V_3 . It would seem therefore that V_2 would be a preferable design criterion to V_3 .

Since V_2 is a measure of the variance per observation per unit area, it can be used to compare the efficiency of different designs and to make recommendations as to how large a design to use. It is important to notice at this point that the minimum integrated variance, V^* , that Box and Draper would get for this problem, using their sufficient conditions to obtain Min B, would be $V^* = 3.0$. This is considered to be an acceptable level of variance. Consequently, when we are comparing the efficiency of various size designs, it is important to realize that all of the designs with $V_2 \leq 3.0$ will be considered

to be acceptable designs. Thus for the SRI, the designs with $N=8$ or $N=9$ are recommended. This is because both of these designs offer more information than just at the center and boundary of the region of interest.

For the CRI the same minimum value of V_2 is obtainable for $N=6, 7,$ and 9 . However, since all three of these designs consist of observations only at the center and at the boundary of the region of interest, an experimenter might want to use the optimal design for $N=8$. The minimum value of V_2 for $N=8$ is 2.648 versus 2.625 for $N=6, 7,$ and 9 . This is a small difference that allows the experimenter to choose a design that is very good and yet does not have the disadvantages discussed before, of designs consisting of only boundary points and center points.

4.2 Designs for Quadratic Polynomials Protecting Against Cubic Effects

In this section several designs are developed that are optimal for the minimum bias quadratic model that protects against a cubic polynomial being the true model (by "protect" it is meant that if the true model is a cubic polynomial, the minimum achievable value of the integrated squared bias B will be achieved by the fitted quadratic model, for any design for which A_{β} is estimable). In two dimensions, these designs will be denoted by

$$(q=2, d=3, k=1). \quad (4.2.1)$$

For the minimum bias quadratic model that protects against cubic effects, only V_2 will be used as a variance criterion for several reasons. Primary among these reasons was the extreme difficulty of determining the relative merit of designs found by using V_1 or V_3 as the variance criterion. There are three basic reasons why such a difficulty arises:

1. Neither V_1 nor V_3 is scaled to make designs of different size comparable.

2. The range of values of V_1 and V_3 for a given design size was so large as to impede the determination as to which designs are good.
3. There was considerable evidence that the optimal designs for V_1 would turn out to be singular designs that could not be approached by a search procedure.

Using V_2 as a variance criterion solved most of these problems. Since V_2 is scaled for both the number of points in the design and for the area of the region of interest, meaningful comparisons between designs are readily available. Using the Box and Draper sufficient conditions to obtain Min B for this problem, would give designs with $V^* = 6.0$. This is considered an acceptable level of average variance and furnishes an excellent method to judge the merit of designs produced. Finally the problem of the optimal designs being singular and unapproachable by a search procedure did not appear in using V_2 . A number of singular designs were tested but none proved to be very good. Consequently, it was decided to consider only V_2 as a variance criterion for the ($q=2$, $d=3$, $k=1$) designs.

Designs with $6 \leq N \leq 13$ have been investigated using V_2 as a variance criterion. Table 7 presents the optimal designs found for a SRI and Table 8 presents the optimal designs found for a CRI. Both tables list designs for $10 \leq N \leq 14$. Smaller designs than $N=10$ exist for which A_{β} is estimable; however, the variance is very high for these small designs. Also designs for $N < 10$ are such that only a particular location for the points allows A_{β} to be estimable. This is unsatisfactory for a search procedure since the answer must be known in order to find it because of the absence of continuity. For this reason the discussion is restricted to designs for which $N \geq 10$. It is also important to note that while an extensive search of designs for $10 \leq N \leq 13$ was conducted, only the best previous patterns were searched for $N=14$.

With the exception of the 10 point design, the optimal designs for a SRI all follow the same pattern of placing one observation in each corner of the region of interest and the rest equally spaced on a circle of radius $\rho_2 \approx .83$. Only the 10 point design is different from this pattern. This difference is due primarily to necessity of $A\beta$ being estimable. The ten point design of the same pattern, i.e., $(4, \frac{\pi}{4}) + (6, 0)$, is such that $A\beta$ is not estimable. This lack of estimability helps to explain the big jump in the value of V_2 between the optimal 10 point design and the optimal 11 point design. From $N=11$ to $N=14$ the change in V_2 is gradual.

It should be noted that there is little change in V_2 due to rotation of the inner circle of these optimal designs. Usually the change is in the seventh or eight decimal for the square region of interest and is even smaller for the circular region of interest. Thus the angles given in Table 7 and Table 8 for the inner circle are not necessarily optimal but are generally chosen for ease in the construction of the design.

The designs in Table 7 allow the experimenter to avoid any difficulties. For $N=11$ he can use a design with only four points on the boundary of his region of interest and the rest well inside of the region of interest. This means that the designs produced will yield information inside the region of interest and not just on the boundary. Also it is important to note that designs with one center point, one point in each of the four corners, and the remaining points equally spaced on a circle of radius $\rho_2 = .83$, are nearly optimal. An experimenter trying to determine the optimal size design to use will obviously be guided by the cost of additional observations. As was mentioned earlier, values of V_2 are comparable as variance per observations per unit area. If observations are free the best thing to do is to take as many observations as is possible. But since observations are rarely free,

the value of V_2 offers a nice comparison between the efficiencies of any two different designs to which the cost of observations can readily be added.

Table 8 of optimal designs found for CRI also shows a distinct pattern. The pattern starts for $N=12$ and holds for larger designs. The pattern is to place an equal number of points (where possible) on two concentric circles, the outer one having radius $\rho_1 = 1$ and the inner one $\rho_2 = .528$ or $.584$ depending upon whether the number of design points is even or odd. If the design size is odd, the remaining point should be placed at the center of the region of interest. This same pattern seems to hold as the optimal designs for larger size designs not included in the table.

However, there appears to be no reason to look at designs larger than $N=14$ since it appears that a lower bound of $V_2 = 5.1384$ has been found. It is interesting to note that we achieve this apparent lower bound for $N=12$ and $N=14$ but cannot achieve it for odd values of N . The fact that designs with N even (and greater than 10) can achieve this value and designs where N is odd cannot may be due to a condition of symmetry. In any case, cost of the observations will probably dictate using $N=12$ since it does achieve this lower bound with the least number of observations.

The simplicity of the optimal designs for both a square and a circular region of interest makes them attractive and should facilitate their use by experimenters. However, there are still problems associated with the use of optimal designs. The optimal designs for the square region of interest are not good configurations to use if the region of interest is circular. In fact, the optimal designs in Table 7 are very poor if scaled and placed in a circular region of interest. The same thing is true if you use the optimal designs from Table 8 when the region of interest is a square. This result is not surprising since each table presents a very definite and different pattern

for the optimal designs. But it does underscore the point made in Section 4.1. The experimenter must know what shape his region of interest is if he wants to use optimal designs.

5. SUMMARY

The minimum bias approach offers the chance to have protection against bias and still enjoy the advantages of variance-optimal design criteria. When a true model, $\eta = \underline{x}'_1 \underline{\beta}_1 + \underline{x}'_2 \underline{\beta}_2$ is approximated by $\hat{y} = \underline{x}'_1 \underline{b}_1$ over a region of interest R , the MBE obtains the same minimum integrated squared bias B for any experimental design for which $A\underline{\beta}$ is estimable. The class of designs for which $A\underline{\beta}$ is estimable contains an infinite number of designs. This flexibility has allowed the construction of D-optimal, V-optimal, and A-optimal experimental designs. There is sufficient flexibility to satisfy other types of design criteria, i.e., orthogonality, rotatability, etc., and still be a near optimal design for any variance criterion, if not the optimal design.

Many areas for further study are implied by these procedures. The minimum bias approach can be applied to problems where the true model is not a polynomial. The approach is also easily extended to any number of dimensions. Allowing the design points to occur outside the region of interest causes no added complications. Constraints upon the achievable values of the independent variables is another area suggested for future study. Thus, the minimum bias approach is a simple procedure for determining good experimental designs in a variety of situations where protection against the inadequacy of the fitted model is of importance to the experimenter,

1. OPTIMAL DESIGNS FOR V_1 ($q=2$, $d=2$, $k=1$, SQUARE REGION OF INTEREST)

N	Designs	N_o	ρ_1	ρ_2	V_1	V_2	V_3
5	$(4, \frac{\pi}{4})$	1	$\sqrt{2}$	-----	33.9*	3.19*	.972*
6	$(4, \frac{\pi}{4})$	2	$\sqrt{2}$	-----	64.0*	2.50*	.750*
7	$(4, \frac{\pi}{4}) + (3, \frac{\pi}{24})$	0	$\sqrt{2}$.020	91.0*	2.40	.676
8	$(4, \frac{\pi}{4}) + (2, \frac{\pi}{4})$	2	$\sqrt{2}$	$\sqrt{2}$	131.7*	2.94	.618
9	$(4, \frac{\pi}{4}) + (2, \frac{\pi}{4})$	3	$\sqrt{2}$	$\sqrt{2}$	189.4*	2.65	.544

2. OPTIMAL DESIGNS FOR V_2 ($q=2$, $d=2$, $k=1$, SQUARE REGION OF INTEREST)

N	Designs	N_o	ρ_1	ρ_2	V_1	V_2	V_3
5	$(4, \frac{\pi}{4})$	1	$\sqrt{2}$	-----	33.9*	3.19*	.972*
6	$(4, \frac{\pi}{4})$	2	$\sqrt{2}$	-----	64.0*	2.50*	.750*
7	$(4, \frac{\pi}{4})$	3	$\sqrt{2}$	-----	91.0	2.40*	.676
8	$(4, \frac{\pi}{4}) + (4, 0)$	0	$\sqrt{2}$.322	121.6	2.43*	.621
9	$(4, \frac{\pi}{4}) + (4, 0)$	1	$\sqrt{2}$.559	164.5	2.47*	.563

3. OPTIMAL DESIGNS FOR V_3 ($q=2$, $d=2$, $k=1$, SQUARE REGION OF INTEREST)

N	Designs	N_o	ρ_1	ρ_2	V_1	V_2	V_3
5	$(4, \frac{\pi}{4})$	1	$\sqrt{2}$	-----	33.9*	3.19*	.972*
6	$(4, \frac{\pi}{4})$	2	$\sqrt{2}$	-----	64.0*	2.50*	.750*
7	$(4, \frac{\pi}{4}) + (3, \frac{\pi}{24})$	0	$\sqrt{2}$.024	90.9	2.40	.676*
8	$(4, \frac{\pi}{4}) + (4, 0)$	0	$\sqrt{2}$.632	127.6	2.56	.597*
9	$(4, \frac{\pi}{4}) + (4, 0)$	1	$\sqrt{2}$.831	173.7	2.62	.538*

*Optimal designs for this type of variance criterion

4. OPTIMAL DESIGNS FOR V_1 ($q=2$, $d=2$, $k=1$, CIRCULAR REGION OF INTEREST)

N	Designs	N_o	ρ_1	ρ_2	V_1	V_2	V_3
5	(4,0)	1	1	----	12.8*	2.813*	1.313*
6	(4,0)	2	1	----	21.3*	2.625*	1.188
7	(5,0)	2	1	----	35.7*	2.625*	.975
8	(6,0)	2	1	----	54.0*	2.667	.833
9	(7,0)	2	1	----	76.2*	2.714	.732*

5. OPTIMAL DESIGNS FOR V_2 ($q=2$, $d=2$, $k=1$, CIRCULAR REGION OF INTEREST)

N	Designs	N_o	ρ_1	ρ_2	V_1	V_2	V_3
5	(4,0)	1	1	----	12.8*	2.813*	1.313*
6	(4,0)	2	1	----	21.3*	2.625*	1.188
7	(5,0)	2	1	----	35.7*	2.625*	.975
8	(5,0) + (3, $\frac{\pi}{24}$)	0	1	.287	49.0	2.648	.903
9	(6,0)	3	1	----	72.0	2.625*	.792

6. OPTIMAL DESIGNS FOR V_3 ($q=2$, $d=2$, $k=1$, CIRCULAR REGION OF INTEREST)

N	Designs	N_o	ρ_1	ρ_2	V_1	V_2	V_3
5	(4,0)	1	1	----	12.8*	2.813*	1.313*
6	(5,0)	1	1	----	20.8	2.800	1.100*
7	(6,0)	1	1	----	30.9	3.208	.958*
8	(6,0) + (2,0)	0	1	.214	52.9	2.715	.832*
9	(7,0)	2	1	----	76.2*	2.714	.732

*Optimal designs for this type of variance criterion

7. OPTIMAL DESIGNS FOR V_2 ($q=2$, $d=3$, $k=1$, SQUARE REGION OF INTEREST)

N	Designs	N_o	ρ_1	ρ_2	V_2
10	$(7, \frac{\pi}{28}) + (3, \frac{\pi}{14})$	0	1.00633	.32551	5.9786
11	$(4, \frac{\pi}{4}) + (7, 0)$	0	$\sqrt{2}$.83152	5.6084
12	$(4, \frac{\pi}{4}) + (8, \frac{\pi}{8})$	0	$\sqrt{2}$.83161	5.4348
13	$(4, \frac{\pi}{4}) + (9, 0)$	0	$\sqrt{2}$.83171	5.3109
14	$(4, \frac{\pi}{4}) + (10, 0)$	0	$\sqrt{2}$.83183	5.2218

8. OPTIMAL DESIGNS FOR V_2 ($q=2$, $d=3$, $k=1$, CIRCULAR REGION OF INTEREST)

N	Designs	N_o	ρ_1	ρ_2	V_2
10	$(7, 0) + (3, 0)$	0	.88447	.37038	5.6270
11	$(6, 0) + (5, 0)$	0	.98732	.50541	5.2663
12	$(6, 0) + (6, \frac{\pi}{6})$	0	1	.52806	5.1384
13	$(6, 0) + (6, \frac{\pi}{6})$	1	1	.58411	5.1864
14	$(7, 0) + (7, \frac{\pi}{7})$	0	1	.52806	5.1384

REFERENCES

1. Box, G. E. P. and N. R. Draper. "A basis for the selection of a response surface design", Journal of the American Statistical Association, (1959), 54:622-654.
2. Box, G. E. P. and N. R. Draper. "The choice of a second order rotatable design", Biometrika, (1963), 50:335-352.
3. Box, G. E. P. and K. B. Wilson. "On the experimental attainment of optimum conditions", Journal of the Royal Statistical Society, Series B, (1951), 13:1-45.
4. Box, M. J. and N. R. Draper. "Factorial designs, the $|X'X|$ criterion, and some related matters", Technometrics, (1971), 13:731-742.
5. Dykstra, O. "The augmentation of experimental data to minimize $|X'X|$ ", Technometrics, (1971), 13:682-688.
6. Evans, J. W. "Computer generated D-optimal, V-optimal, and trace optimal minimum bias experimental designs", Series No. 936, Institute of Statistics, North Carolina State University, 1974 (mimeographed).
7. Fedorov, V. V. The Theory of Optimal Experiments, New York: Academic Press, 1972.
8. Hartley, H. O. and P. G. Ruud. "Computer optimization of second order response surface designs", Proceedings of the Conference of Statistical Computation, University of Wisconsin, April-May, published as Statistical Computation (R.C. Milton and J. A. Nelder, Editors), New York: Academic Press, 1969, 441-462.
9. Hendrix, C. D. "Empirical optimization in research and development", Second Gordon Research Conference on Operation Research and Management Science, Aug. 9-13, 1971, New Hampshire: Holderness, 1971.
10. Karson, M. J., A. R. Manson, and R. J. Hader. "Minimum bias estimation and experimental design for response surfaces", Technometrics, (1969), 11:461-475.
11. Mitchell, T. J. "An algorithm for the construction of "D-optimal" experimental designs", Technometrics, (1974), 16:203-210.
12. Mitchell, T. J. "Computer construction of "D-optimal" first-order designs", Technometrics, (1974), 16:211-220.
13. Stigler, S. M. "Optimal experimental design for polynomial regression", Journal of the American Statistical Association, (1971), 66:311-318.