ResearchGate

See discussions, stats, and author profiles for this publication at: https://www.researchgate.net/publication/241735968

Extreme Vertices Designs for Linear Mixture Models

Article *in* Technometrics · August 1974

DOI: 10.1080/00401706.1974.10489209

CITATIONS
116

READS
1,117

2 authors, including:

Ron Snee
Snee Associates, LLC
435 PUBLICATIONS **8,346** CITATIONS

SEE PROFILE

Some of the authors of this publication are also working on these related projects:

Problem Solving View project

Quality by Design View project

All content following this page was uploaded by Ron Snee on 22 October 2016.

The user has requested enhancement of the downloaded file.

TECHNOMETRICS©, VOL. 16, NO. 3, AUGUST 1974

Extreme Vertices Designs for Linear Mixture Models

Ronald D. Snee and Donald W. Marquardt

Engineering Department
E. I. du Pont de Nemours & Company
Wilmington, Delaware

Extreme vertices designs are useful in experimentation with mixtures, particularly when the response can be described by a linear model. An algorithm is proposed for selecting a subset of extreme vertices when the number of candidate vertices is large. This algorithm has been found to produce designs which generally have small trace $(\mathbf{X}'\mathbf{X})^{-1}$, indicating the average variance of the estimated coefficients in the linear model will be small.

KEY WORDS

Extreme Vertices
Linear Model
Mixture Designs
Mixture Experiments

1. INTRODUCTION

Many products, such as gasoline, concrete, polymer plastics, alloys, ceramics, paints, cake mixes, and textile fiber blends, are manufactured by mixing two or more ingredients or components. In each mixture or blend, the proportions of each of the q components (X_i) in the mixture must satisfy the following mathematical constraints.

$$0 \leq X_i \leq 1.0, \qquad \sum_{i=1}^{q} X_i = 1.0 \qquad (1)$$

The response of a mixture system depends only on the proportions of the components, and not on the total amount of the mixture.

Several authors [3–8, 11, 14, 17, 18, 20–22] have presented designs for mixture experiments. The designs developed by Scheffé [20, 21], Draper and Lawrence [7, 8], and Becker [2] are useful in those situations where all the components can vary from 0 to 1.0; however, in many situations there are additional constraints on some or all of the components. These constraints often result from economic considerations, the physical situation, and/or previous research. The constraint that some or all of the components must lie between some lower (a_i) and upper (b_i) bound

$$0 \leq a_i \leq X_i \leq b_i \leq 1 \qquad i = 1, 2, \cdots, q \qquad (2)$$

occurs often in practice. The objective of this paper is to present some designs which are useful when this type of constraint is imposed on the X_i's, and the response can be described by a linear model.

The designs proposed by Scheffé, Draper and Lawrence, and Becker can be used in this situation if the ranges $(b_i - a_i)$ of the components are all equal and define a simplex when the X_i's are expressed in terms of pseudocomponents [13]. Hackler, *et al.*, [14], Donelson and Wilson [6], and Kenworthy [17] suggested that the q components be defined in terms of $q - 1$ ratios which could be varied independently, using a factorial or response surface design. Thompson and Myers [22] and Cornell and Good [4] developed rotatable designs for those mixture systems where the region of interest is a hyperellipsoid. Both the ratio designs and rotatable designs are not appropriate when the region of interest is an irregular hyperpolyhedron defined by (1) and (2). If used, these designs may cover only a small amount of the available region, and the resulting models will have unnecessarily large average coefficient error.

Another popular procedure encountered in practice is based on the factorial design for independent variables. The levels of the first $q - 1$ components are developed from the levels of the first $q - 1$ factors in a factorial design (usually some form of a two-level design), and the levels of the last component are calculated so the components add to 1.0, $X_q = 1.0 - \sum_{i=1}^{q-1} X_i$. This method sometimes requires the constraints to be adjusted considerably so the factorial design can be used. This can present problems in that some of the adjusted points may not lie in the region of interest and/or there will be no data collected in some parts of the available space.

We seek to develop a practical method of constructing designs that are near optimum; that is, we want practical designs of high efficiency. The best available solution to this problem is to start with the extreme vertices design procedure proposed by McLean and Anderson [18]. Their procedure permits exploration of the entire region of interest by using

Received Jan. 1973; revised Oct. 1973

a design whose points are extreme vertices of the hyperpolyhedron defined by (1) and (2). The extreme vertices are the intersections of the constraint planes $X_i = a_i$, $X_i = b_i$, $i = 1, 2, \cdots, q$; subject to the additional constraint $\sum_{i=1}^{q} X_i = 1.0$. A major drawback of this design method is that the number of points is quite large when $q \geq 5$. McLean and Anderson hint at some ways of reducing the number of points but do not elaborate. Gorman [12] has also pointed out that there can be clusters of points in parts of the experimental region. McLean and Anderson recommended that the centroids of the faces of the hyperpolyhedron be added to the design when needed to support terms in a quadratic model. The centroids are not needed to estimate the coefficients in a linear model and will decrease the G-efficiency of the design ([1] to be defined later) if included.

Elfving [10] has shown that for a given model and experimental region, the candidate points for an optimum design are the extreme points of the "expanded" region generated by the model. An extreme point is a point which cannot be expressed as a convex combination of any other group of points. Elfving's result implies that for a linear mixture model, the optimum design must be a subset of the extreme vertices.

In this paper we will assume that the response can be described adequately by a linear model within the region of interest defined by (1) and (2). We will present a procedure for obtaining a subset of the extreme vertices which will provide precise estimates of the parameters in the linear model. The ultimate size of the design will be a function of the number of parameters in the model, the desired standard error of the estimates, and the available resources.

2. Design Criteria

If we want to obtain estimates of the parameters in the model, $\mathbf{Y} = \mathbf{X}\beta + \varepsilon$, where $\mathbf{Y}$ is the $(n \times 1)$ vector of responses, $\mathbf{X}$ is the $(n \times q)$ design matrix, β is the $(q \times 1)$ vector of unknown coefficients, and ε is the $(n \times 1)$ vector of errors with zero mean and variance $\sigma^2 I$, then the variance-covariance matrix for the estimated parameters $(\hat{\beta})$ is $\sigma^2(\mathbf{X}'\mathbf{X})^{-1}$.

When comparing various experimental designs, it is desirable to use some quantitative criterion. The three most useful criteria are:

(i) minimum $|(\mathbf{X}'\mathbf{X})^{-1}|$
(ii) minimum trace $(\mathbf{X}'\mathbf{X})^{-1}$
(iii) minimum-maximum variance

All of these criteria are decreasing functions of the number of points in the design (n), in the sense that if a point is added to a given design, all three criteria will decrease.

(i) The generalized variance of the paramcter estimates is $\sigma^2|(\mathbf{X}'\mathbf{X})^{-1}|$ and minimizing $|(\mathbf{X}'\mathbf{X})^{-1}|$ is equivalent to minimizing the volume of the confidence ellipsoid for the parameters. The volume of the region covered by the design is also maximized as $|(\mathbf{X}'\mathbf{X})^{-1}|$ is minimized.

(ii) The trace $(\mathbf{X}'\mathbf{X})^{-1}$ is proportional to the sum of the variance of the regression coefficients,

$$\sum_{i=1}^{q} \text{variance } (\hat{\beta}_i) = \sigma^2 \text{ trace } (\mathbf{X}'\mathbf{X})^{-1}$$

and is a measure of the difference (distance) between the vector of estimated coefficients $(\hat{\beta})$ and the vector of population coefficients (β) as shown by the relation

$$E(\hat{\beta} - \beta)'(\hat{\beta} - \beta) = \sigma^2 \text{ trace } (\mathbf{X}'\mathbf{X})^{-1}$$

where E denotes the expectation operator.

(iii) The maximum variance refers to the maximum variance of prediction over the experimental region where the prediction variance at the point $\mathbf{x}$ $(1 \times q$ row vector) is given by $\sigma^2 v$ and $v = \mathbf{x}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}'$.

The trace $(\mathbf{X}'\mathbf{X})^{-1}$ appears to be the most useful criterion for linear mixture models. This criterion provides a direct measure of the uncertainty in the coefficients in the regression model. For example, this is important in gasoline blending problems where the resulting equation (usually linear) will be used in a linear program (LP) to determine optimum blending procedures.

Although we prefer the trace $(\mathbf{X}'\mathbf{X})^{-1}$ criterion, it is helpful to compute all three criteria for all designs. The criteria usually agree; in the sense that a design that is optimum by one criterion will often be optimum by the others. However, any disagreement can be detected if all three criteria are available. Computation of the maximum variance also provides a measure of how close to optimum the design is. Keifer and Wolfowitz [15] have shown that a design is optimum if the number of parameters in the model (p) is equal to the number of observations in the design (n) times d, where d is the maximum value of $v = \mathbf{x}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}'$ over the experimental region. The G-efficiency (G for global) of the design is given by,

$$\text{G-efficiency (percent of optimum)} = 100\ p/nd.$$

In a linear mixture model, $p = q$. Atwood [1] has shown that G-efficiency $\leq$ D-efficiency, where D-efficiency is based on minimizing $|(\mathbf{X}'\mathbf{X})^{-1}|$. G-efficiency $(100\ q/nd)$ is on a per point basis and is independent of n. As noted earlier, the determinant, trace, and minimum-maximum variance criteria are decreasing functions of n. For a given design, we shall refer to the values of these three criteria as the "design statistics".

Efficiency is an important design concept in this instance. Given a set of N candidate points, there is at least one design of size n which has best design statistics among designs of size n. However, there may be several different designs with the same design statistics as a given design; furthermore, there may be additional designs of size n which are almost as good as a best design. We want a procedure which will consistently produce designs which are close to the best. Our experience has been that, at the present time, optimum designs (G-efficiency = 100%) are expensive to compute and often require large n due to uneven replication of the design points, thereby increasing the cost of experimentation.

As an example, Wynn [24] gives an optimum design for the three-parameter model,

$$E(y) = \beta_0 + \beta_1 X_1 + \beta_2 X_2$$

The four-point design: (2, 2), (−1, 1), (1, −1), (−1, −1) required 32 experiments allocated as follows: 10, 9, 9, 4.

The four point design with a single observation at each point has a G-efficiency of 84%. An additional 28 replicate experimental points are required to reach the exact relative weighting for optimum (G-efficiency = 100%). Wheeler [23] has noted that there is little practical distinction between designs with G-efficiencies of 50 and 80%. In our judgment, any evenly replicated design with a G-efficiency of 50% or better is "optimum" from a practical point of view.

Optimum design theory also tells us that an optimum design for a q parameter linear model would contain, at most, a few more than q distinct points. These points may have unequal replication. Replication has inherent usefulness in providing a measure of experimental error. However, from a practical point of view, a design should also provide a measure of lack of fit, and enable the analyst to detect abnormal observations. Additional distinct points beyond those required by the" optimum" design should be included to obtain this additional information.

3. Selecting Subsets of Extreme Vertices for Linear Models

Any algorithm for selecting subsets of extreme vertices should produce designs which are good with respect to criteria (i), (ii), and (iii) described in Section 2, and have sufficient observations to measure lack of fit and detect abnormal results. The algorithm should also have the property of short run times when programmed on a computer, thereby making the procedure economical to use. The spirit of all such algorithms should be to *aid* in selecting a design, not to dictate a design. Thus, for a given problem, several computer runs may be made before a final design is chosen, thereby making cost per computer run an important factor.

3.1. All Possible Combinations

One possible method of choosing a design of size n from N candidate points would be to compute the trace $(\mathbf{X}'\mathbf{X})^{-1}$ (plus other design statistics as desired) for all possible $\binom{N}{n}$ designs of size n. It would also be desirable to try different n's to determine the effect of sample size on the design characteristics. Such a procedure gives an exact solution to the problem; however, one soon finds that the total number of candidate designs increases so rapidly as N and n increase that this procedure is practical only for small q, say $q \leq 4$.

3.2 CADEX

A second procedure which has possibility is the Computer Aided Design of Experiments algorithm, CADEX for short, developed by Kennard and Stone [16]. The philosophy of CADEX is: given a set of candidate points which cover the feasible experimental region, a good experimental design is that set of points which uniformly cover the available region. Since no model is assumed, optimality of the resulting design is not a direct criterion. CADEX begins by picking the two points which are farthest apart and then adds subsequent points which are farthest from the points already in the design. We find that in mixture problems, the use of McLean and Anderson's standardized distance

$$d_{ij} = \sum_{k=1}^{q} [(X_{ik} - X_{jk})/(b_k - a_k)]^{\frac{1}{2}}$$

often produces better designs (smaller $|(\mathbf{X}'\mathbf{X})^{-1}|$ and tr $(\mathbf{X}'\mathbf{X})^{-1}$ statistics) than the standardization procedure recommended by Kennard and Stone. All CADEX results reported in this paper are based on McLean and Anderson's standardized distance. Because of the selection procedure, CADEX might produce near optimum designs for linear models. Experience has shown that this is the case; however, improvement is still possible. CADEX designs are poorest when the mixture space is tightly constrained.

In Section 4, we describe an algorithm (XVERT) for the computation of extreme vertices. This algorithm not only generates the extreme vertices, but also can be used to select a subset of the extreme vertices. XVERT has been found to produce designs which generally have smaller trace $(\mathbf{X}'\mathbf{X})^{-1}$ than designs produced by CADEX. Illustrative examples are included in Sections 5–7.

4. The XVERT Algorithm

McLean and Anderson recommended that the extreme vertices be computed by forming all possible combinations (two-level factorial design) of the upper (b_i) and lower (a_i) limits of the first $q - 1$ components and then computing the level of the qth component. A given point is an extreme vertex if the computed value for X_q lies on or between the lower (a_q) and upper (b_q) limits of X_q, $a_q \leq X_q \leq b_q$. This procedure produces 2^{q-1} possible points. The process is repeated q times allowing each X to be the variable whose levels are computed. This algorithm produces a total of $N = q2^{q-1}$ possible points, many of which may not fall in the constrained region.

The extreme vertices also can be computed using the XVERT algorithm described below.

(i) Rank the components in order of increasing ranges ($b_i - a_i$): X_1 has the smallest range, and X_q has the largest range.

(ii) Form a two-level design from the upper and lower bounds of the $q - 1$ components with the smallest ranges.

(iii) Compute the level of the qth component

$$X_q = 1.0 - \sum_{i=1}^{q-1} X_i$$

(iv) A given point is an extreme vertex if $a_q \leq X_q \leq b_q$. For those points which are outside of the constraint limits, set X_q equal to the upper or the lower limit, whichever is closest to the computed value.

(v) From each point originally outside of the limits, generate additional points (max = $q - 1$) by adjusting the level of one component by an amount equal to the difference between the computed value for X_q and the substituted upper or lower limit. Additional points are generated only from those components whose adjusted levels will remain within the limits of the components.

There are 2^{q-1} original points, and each point can generate at most $q - 1$ additional points, resulting in a total of $2^{q-1} + (q - 1)2^{q-1}$ possible points. Points are not computed if the levels of at least one X fall outside the constraints. Further, there are often replicate points which must be omitted. Replicates can occur only when the last component X_q is at its highest (b_q) or lowest (a_q) level. Thus, only two sets of points have to be checked for replicates.

In addition to being faster computationally than the McLean and Anderson algorithm, XVERT can also be adapted to generate an efficient experimental design for the linear mixture model

$$E(y) = \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_q X_q$$

The points in the design are the subset of extreme vertices computed from a 2^{q-1} design as described below.

(i) Compute the level of X_q for all points.

(ii) All points where $a_q \leq X_q \leq b_q$ form the *core* of the design.

(iii) Each point whose level of X_q has to be adjusted creates additional points which form a *candidate subgroup.*

(iv) *The design will consist of the core points and one point from each candidate subgroup.* In a given subgroup, the point which is included in the best design is determined by forming all possible combinations of the core points and one point from each subgroup. If n_i = number of points in the ith subgroup, then the total number of possible designs is $\prod_{i=1}^{k} n_i$ where k = number of subgroups.

(v) The trace $(\mathbf{X'X})^{-1}$, $|(\mathbf{X'X})^{-1}|$, and G-efficiency statistics are computed for each design, and those designs with minimum $|(\mathbf{X'X})^{-1}|$, trace $(\mathbf{X'X})^{-1}$, and maximum G-efficiency are determined.

The number of points in the resulting design, is at most, the number of points in the design used to generate the core points and candidate subgroups. It is not always possible to adjust all points with $X_q < a_q$ or $X_q > b_q$. A 2^{q-1} design, which generates all the extreme vertices, will have a large number of points when $q \geq 6$. The number of points in the design can be reduced by using a fraction of a 2^{q-1} design and/or using the first $q - 1$ columns of a Plackett-Burman design [19]. These designs exist for $n = 4, 8, 12, 16, 20$, etc. The effect of n on the design statistics can be determined by constructing designs for 2 or 3 values of n using the Plackett-Burman and two-level fractional factorial designs (eg., $q = 5$, construct designs for $n = 12$, 16 and 20).

This basic algorithm works well in practice except in those situations where the number of candidate subgroups and/or number of points per subgroup is large producing an unrealistic number of candidate designs to be evaluated and excessive computer run times.

The number of points in the candidate subgroups is reduced, as part of the XVERT algorithm, by noting that in the case of the linear model, the trace $(\mathbf{X'X})^{-1}$ is increased most by those X_i's with the smallest ranges. Thus, we would like those X_i's to appear in the design at their high and low levels only. This suggests that the size of the candidate subgroups can be reduced by omitting any point which does not appear at the high or low level for those X's with the smallest ranges.

We begin by looking at the variable with the smallest range, second smallest range, etc., and

eliminating points until $\prod_{i=1}^{k} n_i$ is less than some specified number which we know will produce acceptable computer times. The only constraint is that there is at least one point in each subgroup.

5. Three-Component Example

To begin, consider the following three-component example.

Component	Minimum (a)	Maximum (b)	Range (b − a)
C1	.1	.7	.6
C2	.0	.7	.7
C3	.1	.6	.5

The components ranked in order of increasing ranges are:

Component	Minimum (a)	Maximum (b)	Range (b − a)
X_1 = C3	.1	.6	.5
X_2 = C1	.1	.7	.6
X_3 = C2	.0	.7	.7

The core points are generated by using levels of a $2^{q-1} = 2^{3-1} = 2^2$ factorial design to determine the levels of the first $q - 1 = 3 - 1 = 2$ factors, and the level of $X_q = X_3$ is given by

$$X_3 = 1.0 - \sum_{i=1}^{q-1} X_i = 1.0 - X_1 - X_2$$

The resulting points are:

Point	X_1	X_2	X_3
A	.1	.1	.8
B	.6	.1	.3
C	.1	.7	.2
D	.6	.7	−.3

Points B and C have X_3 = .3 and .2, respectively. These values are within the 0–.7 range specified for X_3 ; however, the levels of X_3 for points A and D (X_3 = .8 and −.3, respectively) are not in the range specified for X_3 . Points A and D must be adjusted to meet the constraint on X_3 . Point A will have X_3 reduced by .1 to .7, the upper constraint on X_3 , and Point D will have X_3 increased by .3 to 0, the lower constraint on X_3 . Both X_1 and X_2 for both points can be adjusted to compensate for the alteration of X_3 .

Point	X_1	X_2	X_3	Adjustment
A	.1	.1	.8	
A1	.1	.2	.7	+.1
A2	.2	.1	.7	+.1
D	.6	.7	−.3	
D1	.6	.4	0	−.3
D2	.3	.7	0	−.3

Each point produces two additional points resulting in a total of six extreme vertices (Figure 1).

Point	Vertex	X_1	X_2	X_3
B	1	.6	.1	.3
C	2	.1	.7	.2
A1	3	.1	.2	.7
A2	4	.2	.1	.7
D1	5	.6	.4	0
D2	6	.3	.7	0

If we were interested in obtaining a 4-point design, then points A and D would generate two candidate subgroups of two points each.

The design would consist of vertices 1, 2, (3 or 4), and (5 or 6). The design statistics (trace $(\mathbf{X}'\mathbf{X})^{-1}$, $|(\mathbf{X}'\mathbf{X})^{-1}|$, G-efficiency) are computed for each of the 4 designs.

Design	Vertex	$\lvert(\mathbf{X}'\mathbf{X})^{-1}\rvert$	tr $(\mathbf{X}'\mathbf{X})^{-1}$	G-Efficiency
1	1, 2, 3, 5	5.88*	6.41*	82
2	1, 2, 3, 6	6.26	6.98	74
3	1, 2, 4, 5	5.97	6.47	81
4	1, 2, 4, 6	6.94	7.83	65

* minimum

It is clear that design 1 with vertices 1, 2, 3, and 5 is the best design. This is the same design that is found to be the best when all possible $\binom{6}{4} = 15$ four-point designs were evaluated. This is also the design chosen by CADEX. In conclusion, all three procedures produce the same design, which is the best available four-point design for the linear model. The following four-component example shows some disagreement between the different algorithms.

6. Four-Component Example

This four-component example is presented because the number of extreme vertices is small, and all possible designs of size n can be evaluated. The ranges of the components in this example are:

Component	Minimum (a)	Maximum (b)	Range (b − a)
X_1	.00	.04	.04
X_2	.00	.10	.10
X_3	.40	.55	.15
X_4	.40	.60	.20

The resulting 10 extreme vertices and designs for $n = 4$ and 8 points are summarized in Tables 1 & 2.

The levels of X_1, X_2, and X_3 in the $n = 4$ design were generated from a 2^{3-1} design with alias $X_3 = X_1X_2$.

Point	Vertex	X_1	X_2	X_3	X_4
A	5	0	0	.55	.45
B	3	.04	0	.40	.56
C	2	0	.10	.40	.50
D		.04	.10	.55	—
D1	8	.04	.10	.46	.40
D2	10	.04	.01	.55	.40

The computed value for X_4 was within limits for the first three points. Point D could be adjusted in two ways (reduce X_3 by .09 and increase X_4 by .09 or reduce X_2 by .09 and increase X_4 by .09), hence, there are two possible designs: vertices 2, 3, 5, and 8 and 2, 3, 5, and 10.

The levels of X_1, X_2, and X_3 in the 8-point design were generated from a 2^3 design. Two points had X_4 out of limits. Each point could be adjusted in two ways producing a total of $2 \cdot 2 = 4$ possible designs.

For $n = 4$, evaluation of all possible designs indicated that vertices 1, 4, 6, and 7 were the minimum determinant and maximum G-efficiency (81%) designs. Vertices 2, 3, 5, and 8 were the minimum trace design with G-efficiency = 62%. The XVERT algorithm produced the minimum trace design. The CADEX design (vertices 1, 2, 8, and 9) had a G-efficiency of 28%.

It is interesting to note that using the alias

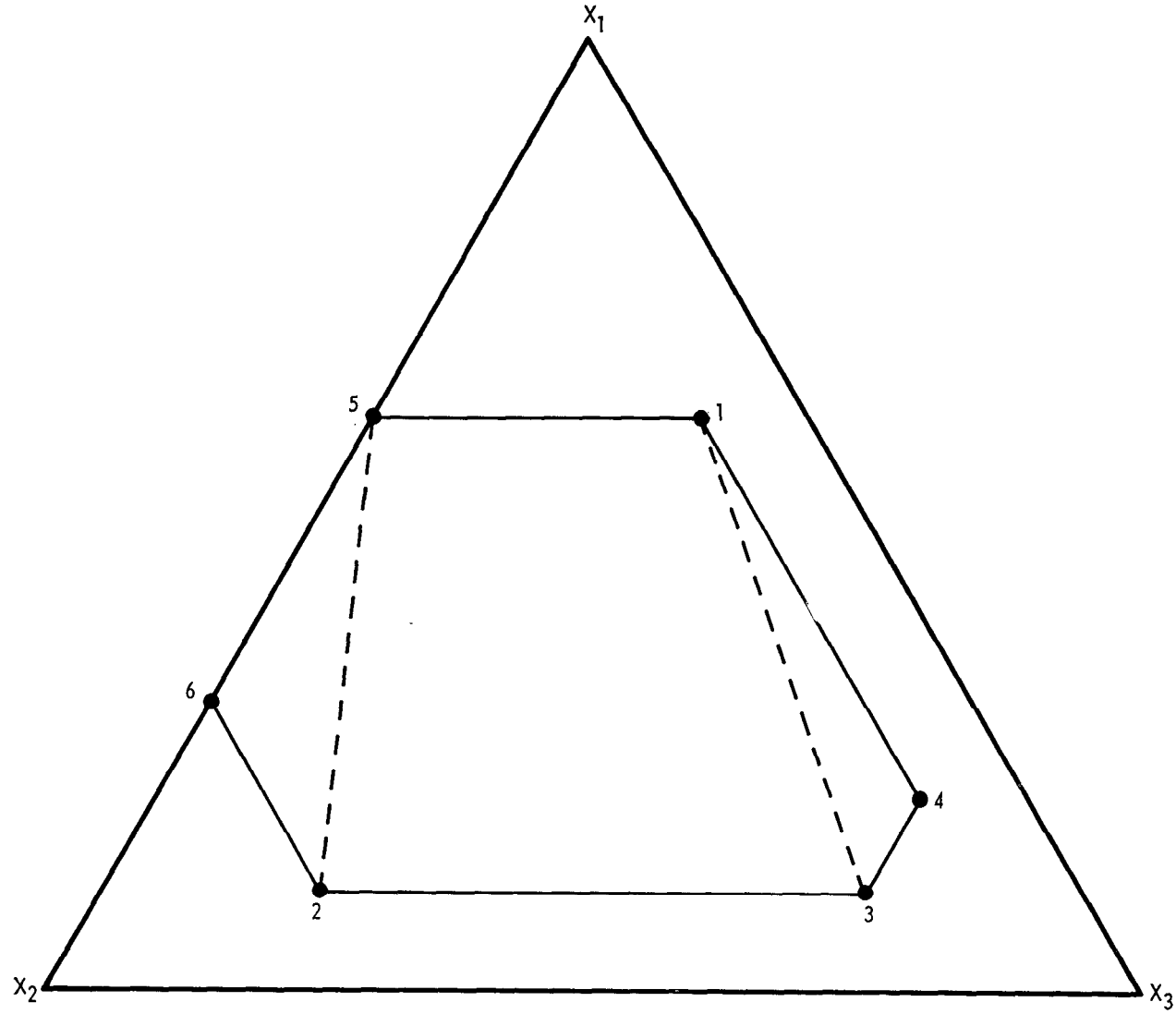

FIGURE 1—Three Component Example Experimental Region Best Four-Point Design is Vertices 1, 2, 3 and 5

$X_3 = -X_1X_2$, XVERT produced two four-point designs: vertices 1, 4, 6, and 7 and 1, 4, 6, and 9. We noted earlier the design with vertices 1, 4, 6, and 7 had the smallest determinant and the largest G-efficiency of all possible four-point designs.

For $n = 8$, evaluation of all possible designs indicated that vertices 1–8 made up the minimum determinant, trace, and maximum G-efficiency (88%) designs. The XVERT algorithm also produced vertices 1–8, while CADEX selected vertices 1–3, 5–9 with G-efficiency = 72%.

In this example, XVERT produced the best possible designs for one or more of the optimality criteria. We have observed similar results in other examples where it was practical to evaluate all possible designs. The next example illustrates the performance of the XVERT algorithm on problems with large numbers of extreme vertices.

7. Five-Component Example

The objective of a gasoline blending study was to develop a blending model for a five-component system with the following component ranges:

Component	Minimum (a)	Maximum (b)	Range (b − a)
X_1 = Butane	.00	.10	.10
X_2 = Alkylate	.00	.10	.10
X_3 = Lt. St. Run	.05	.15	.10
X_4 = Reformate	.20	.40	.20
X_5 = Cat Cracked	.40	.60	.20

Prior experience indicated that a linear model would give an adequate description of the gasoline research octane (y) over these ranges. In addition to obtaining precise estimates of the coefficients in the model (blending values), it was also desirable to include enough observations to obtain a measure of a model residual standard deviation (lack of fit plus observation error) and have the ability to detect abnormal observations which are often indicative of blending and/or rating errors. It was concluded that a 16-point design, which would have 11 degrees of freedom to estimate the residual standard deviation, would be sufficient to accomplish these objectives.

Table 1—*Four-Component Example Extreme Vertices*

Vertex	X_1	X_2	X_3	X_4
1	.00	.00	.40	.60
2	.00	.10	.40	.50
3	.04	.00	.40	.56
4	.04	.10	.40	.46
5	.00	.00	.55	.45
6	.04	.00	.55	.41
7	.00	.10	.50	.40
8	.04	.10	.46	.40
9	.00	.05	.55	.40
10	.04	.01	.55	.40

The core points and candidate subgroup points for the XVERT design are shown in Table 3. In this case, all 28 extreme vertices are included in the core points and candidate subgroup points. The 6 candidate subgroups each contain 3 points; hence, there are $3^6 = 729$ designs to be evaluated. Here, the minimum determinant, minimum trace and maximum efficiency designs turn out to be the same design. The statistics for this 16-run design (core

Table 2—*Four-Component Example Design Statistics*

n	Algorithm	Vertices	$\lvert (X'X)^{-1} \rvert$	$\mathrm{tr}\,(X'X)^{-1}$	G-Efficiency
4	All Possible Combinations	1,4,6,7	10×10^5 *	804	81
	XVERT	2,3,5,8	14×10^5	774*	62
	CADEX	1,2,8,9	28×10^5	1417	28
8	All Possible Combinations	1-8	66×10^3 *	366*	88
	XVERT	1-8	66×10^3*	366*	88
	CADEX	1-3, 5-9	74×10^3	405	72

* minimum

points plus vertices 11, 14, 17, 20, 23, 26) and the 16-run CADEX design are:

Design	$\lvert(\mathbf{X}'\mathbf{X})^{-1}\rvert$	tr $(\mathbf{X}'\mathbf{X})^{-1}$	G-Efficiency
XVERT	14×10^3	75	95
CADEX	23×10^3	102	53

It is clear that the XVERT design is considerably better than the CADEX design. The difference between the designs of the two algorithms is not always this large. It is not practical to determine the optimum 16-run design by examining all possible cases. That would require the evaluation of $\binom{28}{16} = 30{,}421{,}755$ designs.

In this example, the XVERT design was developed from the first four columns of the 16-run Plackett-Burman design which is identical to a 2^4 factorial design. It is interesting to note that the XVERT design included the first point from each of the candidate subgroups. In other examples, the core points plus first point from each subgroup has been found to be close to, if not, the minimum trace design.

The five coefficient (coefficient standard errors in parentheses) linear model

$$\hat{y} = \underset{(1.5)}{102.4X_1} + \underset{(1.5)}{100.7X_2} + \underset{(1.4)}{85.2X_3} + \underset{(0.7)}{84.7X_4} + \underset{(0.5)}{97.6X_5}$$

fit the 16 observed research octane numbers (Table 3) with a residual standard deviation of 0.32. The research octane rating error was known to be approximately 0.30. The ratio, (residual variance)/σ^2 = $(0.32)^2/(0.30)^2$ = 1.14, has a χ^2 distribution with 11 degrees of freedom. It was concluded that the lack of fit was not statistically significant and

TABLE 3—*Five-Component Example*

Group		Vertex	X_1 Butane	X_2 Alkylate	X_3 LSR***	X_4 Reformate	X_5 CC***	y Octane**
Core Points *		1	.10	.10	.05	.20	.55	95.1
		2	.10	.00	.15	.20	.55	93.4
		3	.00	.10	.15	.20	.55	93.3
		4	.10	.10	.15	.20	.45	94.1
		5	.00	.00	.05	.40	.55	91.8
		6	.10	.00	.05	.40	.45	91.8
		7	.00	.10	.05	.40	.45	92.5
		8	.00	.00	.15	.40	.45	90.5
		9	.00	.00	.05	.35	.60	92.7
		10	.10	.10	.15	.25	.40	93.5
Candidate Subgroup	1	11 *	.10	.00	.05	.25	.60	94.8
		12	.10	.00	.10	.20	.60	
		13	.10	.05	.05	.20	.60	
	2	14 *	.00	.10	.05	.25	.60	93.7
		15	.00	.10	.10	.20	.60	
		16	.05	.10	.05	.20	.60	
	3	17 *	.00	.00	.15	.25	.60	92.5
		18	.00	.05	.15	.20	.60	
		19	.05	.00	.15	.20	.60	
	4	20 *	.10	.10	.05	.35	.40	93.1
		21	.10	.05	.05	.40	.40	
		22	.05	.10	.05	.40	.40	
	5	23 *	.10	.00	.15	.35	.40	91.8
		24	.10	.00	.10	.40	.40	
		25	.05	.00	.15	.40	.40	
	6	26 *	.00	.10	.15	.35	.40	91.6
		27	.00	.10	.10	.40	.40	
		28	.00	.05	.15	.40	.40	

* XVERT $\lvert(\mathbf{X}'\mathbf{X})^{-1}\rvert$, tr$(\mathbf{X}'\mathbf{X})^{-1}$, and maximum efficiency design. CADEX design is vertics 9, 10, 12–19, 21, 22, 24, 25, 27, 28.

** Research Octane at 2.0 gmPb/gal.

*** Light Straight Run, cat cracked.

the linear model gave an adequate description of the research octane within the region of these data. A residual analysis did not detect any abnormal data points.

8. Concluding Remarks

Experience has shown that extreme vertices designs [18] are useful in studying the response of a mixture system in which the components have upper and lower constraints. These designs contain large numbers of points [12]. These problems can be eliminated by selecting a subgroup of extreme vertices. In this paper, we have proposed a new algorithm, XVERT, for selecting a subset which generally gives better designs, in terms of the trace $(\mathbf{X}'\mathbf{X})^{-1}$, than the CADEX algorithm [16] which was proposed for the general design problem (both physical and mathematical constraints). It should be noted, however, the CADEX can provide a design for any $q \leq n \leq N$, while XVERT is restricted to the number of points in the two-level design used to generate the core points and candidate subgroups.

XVERT has the additional advantage of not computing all extreme vertices, which can itself be quite time consuming for large problems. For example, 10 component problems typically have around 1000 extreme vertices while 15 component problems may have 2000 or more vertices. Gasoline blending problems with 10–15 components are not uncommon. Algorithms [9, 16, 24] which search all possible extreme vertices become impractical for these large problems. Also, some optimization algorithms [24] need a set of points to start with.

Table 4—*XVERT Design G-Efficiencies*

Sample Problem	q	N	n	Design Criteria *	G-Efficiency XVERT Subset	G-Efficiency All Vertices	Δ
A	4	10	4	Det, Tr	62	62	0 **
			8	Det, Tr	84	84	0
B	5	20	8	Det, Tr	84	84	0
			11	Det, Tr	77	76	1
			16	Det, Tr	88	88	0
C	5	28	8	Det, Tr	83	83	0
			12	Det	71	71	0
			12	Tr	63	63	0
			16	Det, Tr	95	95	0
D	6	49	8	Det, Tr	78	63	15 **
			12	Det, Tr	79	79	0
			16	Det	82	74	8
			16	Tr	79	79	0
			20	Det, Tr	77	76	1
E	6	60	7	Det	84	49	35 **
			7	Tr	84	51	33 **
			11	Det, Tr	79	75	4
			19	Det	78	77	1
			19	Tr	78	77	1
F	6	36	9	Det	59	59	0
			9	Tr	60	60	0
			11	Det	51	46	5
			11	Tr	52	49	3
			14	Det	77	77	0
			14	Tr	64	59	5
G	7	109	8	Det, Tr	76	59	17 **
			12	Det	70	70	0
			12	Tr	77	70	7
			16	Det	69	68	1
			16	Tr	71	70	1

* Det = minimum determinant design; Tr = minimum trace design; Det, Tr denotes design had both minimum determinant and minimum trace.

** Nearly Saturated Designs

The XVERT subset is an excellent starting set which is easy to compute.

When choosing a subset of points from a candidate list, we would like the subset to cover as much of the region as possible. A feel for how well a design covers a region can be obtained by comparing the G-efficiency of the design computed over the design points with the G-efficiency of the design computed over the entire candidate list. We have made this type of comparison for 30 designs developed for 7 sample problems using Plackett-Burman designs. The results summarized in Table 4 indicate that the difference in G-efficiency is generally less than 10% with the exception of the nearly saturated designs ($n \approx q$). We conclude that in addition to having small trace $(\mathbf{X}'\mathbf{X})^{-1}$ values, on a per point basis, the XVERT designs cover the major portion of the available experimental region.

Finally, it should be pointed out that the XVERT designs can be augmented to estimate the coefficients in a quadratic model by adding a subset of the centroids of the faces of the hyperpolyhedron to the design. The construction of designs for quadratic models in constrained mixture spaces will be discussed in a later paper.

9. Acknowledgments

The authors wish to express their sincere appreciation to R. W. Kennard and R. E. Wheeler for many useful discussions concerning algorithms for efficient experimental design and to W. E. Morris for bringing the gasoline blending problem to their attention. Appreciation is also expressed to L. W. Scarborough, L. J. Scarborough, S. K. Acuff, L. W. Barracliff, R. E. Boutin, S. V. Furio, and M. H. Sarner for their assistance in writing the computer programs associated with this work and to the referees for their helpful suggestions on the presentation of this paper.

References

[1] Atwood, C. L. (1969). Optimal and efficient designs of experiments. *Ann. Math. Statist., 40,* 1570–1602.

[2] Becker, N. G. (1970). Mixture designs for a model linear in the proportions. *Biometrika, 57,* 329–338.

[3] Claringbold, P. J. (1955). Use of the simplex design in the study of the joint action of related hormones. *Biometrics, 11,* 174–185.

[4] Cornell, J. A. and Good, I. J. (1970). The mixture problem for categorized components. *J. Am. Stat. Assn., 65,* 339–355.

[5] Cornell, J. A. (1971). Process variables in the mixture problem for categorized components, *J. Am. Stat. Assn., 66,* 42–48.

[6] Donelson, D. H. and Wilson, J. T. (1960). Effect of relative quantity of flour fractions on cake quality. *Cereal Chemistry, 37,* 241–262.

[7] Draper, N. R. and Lawrence, W. L. (1965). Mixture designs for three factors, *J. R. Statist. Soc., B27,* 450–465.

[8] Draper, N. R. and Lawrence, W. L. (1965). Mixture designs for four factors, *J. R. Statist. Soc., B27,* 473–478.

[9] Dykstra, O. (1971). The augmentation of experimental data to maximize $|\mathbf{X}'\mathbf{X}|$, *Technometrics, 13,* 682–688.

[10] Elfving, G. (1952). Optimum allocation in linear regression theory, *Ann. Math. Statist., 23,* 255–262.

[11] Gorman, J. W. and Hinman, J. E. (1962). Simplex lattice designs for multicomponent systems, *Technometrics, 4,* 463–487.

[12] Gorman, J. W. (1966). Discussion of "extreme vertices design of mixture experiments" by R. A. McLean and V. L. Anderson, *Technometrics, 8,* 455–456.

[13] Gorman, J. W. (1970). Fitting equations to mixture data with restraints on compositions. *J. Quality Technology, 2,* 186–194.

[14] Hackler, W. C., Kriegel, W. W. and Hader, R. J. (1956). Effect of raw material ratios on absorption of whiteware compositions. *J. American Ceramic Society, 39,* 20–25.

[15] Keifer, J. and Wolfowitz, J. (1960). The equivalent of two extremum problems. *Can. J. Math., 12,* 363–366.

[16] Kennard, R. W. and Stone, L. (1969). Computer aided design of experiments, *Technometrics, 11,* 137–148.

[17] Kenworthy, O. O. (1963). Factorial experiments with mixtures using ratios, *Industrial Quality Control XIX,* No. 12, 24–26.

[18] McLean, R. A. and Anderson, V. L. (1966). Extreme vertices design of mixture experiments. *Technometrics 8,* 447–456.

[19] Plackett, R. L. and Burman, J. P. (1946). The design of optimum multifactorial experiments, *Biometrika, 33,* 305–325.

[20] Scheffé, H. (1958). Experiments with mixtures, *J. R. Statist. Soc., B20,* 344–360.

[21] Scheffé, H. (1963). The simplex-centroid design for experiments with mixtures, *J. R. Statist. Soc., B25,* 235–263.

[22] Thompson, W. O. and Myers, R. H. (1968). Response surface designs for experiments with mixtures. *Technometrics, 10,* 739–756.

[23] Wheeler, R. E. (1972). Efficient experimental design. Submitted for publication.

[24] Wynn, H. P. (1970). The sequential generation of D-optimum experimental designs. *Ann. Math. Statist., 41,* 1655–1664.

View publication stats