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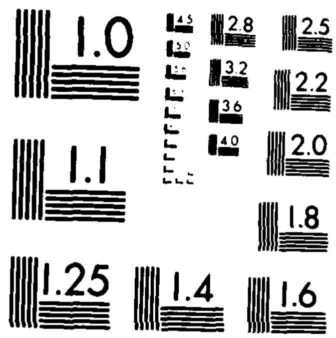
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RESPONSE SURFACE DESIGNS

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ABSTRACT

The fitting of first and second degree equations to experimental data in order to summarize the main features of the underlying but unknown mechanism, is a useful and widely used technique. In addition to its interpretive value, it often provides information about the mechanism. Certain ways of obtaining the data are better than others. Criteria for choice of a suitable response surface design, and specific designs that have excellent characteristics with respect to those criteria, are described in this expository article. Various other related features, suggestions for further reading, and a list of basic references are included.

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RESPONSE SURFACE DESIGNS

Norman R. Draper

Suppose we have a set of observations $y_u, \xi_{1u}, \xi_{2u}, \ldots, \xi_{ku}$, $u = 1,2,\ldots,n$, taken on a response variable y and on k predictor variables $\xi_1, \xi_2, \ldots, \xi_k$. A response surface model is a mathematical model fitted to y as a function of the ξ's in order to provide a summary representation of the behaviour of y. Two basic types of models can be fitted to data arising from a response-predictor relationship:

(a) Empirical models. These are typically models linear in the parameters, often polynomials, either in the basic predictor variables or in transformed entities constructed from these basic predictors. The purpose of fitting empirical models is to provide a mathematical French curve which will summarize the data. (The mechanism that produced these data is, in this context, either unknown or poorly understood.) This article will be concerned only with design of experiments for such empirical models.

(b) Mechanistic models. When knowledge of the underlying mechanism that produced the data is available, it is often possible to construct a model that, reasonably well, represents that mechanism. Such a model is preferable to an empirical one, because it usually contains fewer parameters, fits the data better, and extrapolates more sensibly. (Polynomial models often extrapolate poorly.) However, mechanistic models are often nonlinear in the parameters, and more difficult to fit and evaluate. Also the choice of an experimental design presents intricate problems. For basic information on designs for mechanistic models see the encyclopedia articles "Nonlinear

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Models" and "Nonlinear Regression" and the references therein. A cornerstone article on nonlinear experimental design is by Box and Lucas (1959).

We now continue with (a). Typically, when little is known of the nature of the true underlying relationship, the model fitted will be a polynomial in the ξ's. (The philosophy is that we are approximating the true but unknown surface by low order terms in its Taylor's series* expansion. The words "order" and "degree" are interchangeable in response surface work, and the choice of one word over the other is a matter of personal preference.) Most used in practice are polynomials of first order and second order. The first order model is

$$y_u = \beta_0' + \beta_1'\xi_{1u} + \beta_2'\xi_{2u} + \cdots + \beta_k'\xi_{ku} + \varepsilon_u \tag{1}$$

where it is usually tentatively assumed that the errors $\varepsilon_u \sim N(0,\sigma^2)$ and are independent. The second order model contains additional terms

$$\beta_{11}'\xi_{1u}^2 + \beta_{22}'\xi_{2u}^2 + \cdots + \beta_{kk}'\xi_{ku}^2 + \beta_{12}'\xi_{1u}\xi_{2u} + \cdots + \beta_{k-1,k}'\xi_{k-1,u}\xi_{ku} . \tag{2}$$

Polynomial models of order higher than two are rarely fitted, in practice. This is partially because of the difficulty of interpreting the form of the fitted surface which, in any case, produces predictions whose standard errors are greater than those from the lower order fit, and partly because the region of interest is usually chosen small enough for a first or second order model to be a reasonable choice. Exceptions occur in meteorology where quite high order polynomials have been fitted, but there only two or three ξ's are commonly used. When a second order polynomial is not adequate, and often even when it is, the possibility of making a simplifying transformation in y or in one or more of the ξ's would usually be explored before reluctantly proceeding to higher order, because more parsimonious representations involving fewer terms are generally more desirable. In actual applications, it is common practice to code the ξ's via $x_{iu} = (\xi_{iu} - \xi_{i0})/S_i$,

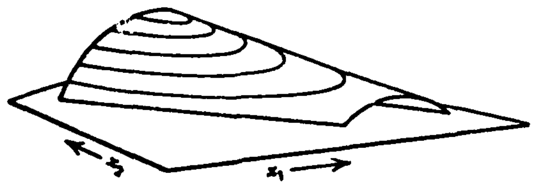
$i = 1,2,\ldots,k$, where ξ_{i0} is some selected central value of the ξ_i-range to be explored, and S_i is a selected scale factor. For example, if a temperature (T) range of 140°C to 160°C is to be covered using three levels 140°C, 150°C, 160°C, the coding $x = (T-150)/10$ will code these levels to $x = -1, 0, 1$ respectively. The second order model would then be recast as

$$y_{iu} = \beta_0 + \beta_1 x_{1u} + \cdots + \beta_k x_{ku} + \beta_1 x_{1u}^2 + \cdots + \beta_k x_{ku}^2$$
$$+ \beta_{12} x_{1u} x_{2u} + \cdots + \beta_{k-1,k} x_{k-1,u} x_{ku} + \varepsilon_u \qquad (3)$$

and would usually be fitted by least squares* in that form. Substitution of the coding formulas into (3) enables the β''s to be expressed in terms of the β's.

What sorts of surfaces are representable by a model of form (3)? Figure 1 shows, for $k = 2$, one basic type which occurs frequently in practice. The three dimensional upper portion of Figure 1 shows a rising ridge, while the lower portion shows the contours of that ridge in the (x_1, x_2) plane. The details of the specific example used are in the figure caption. A change of origin and a rotation of axes brings the fitted equation into the so-called canonical form (in X_1 and X_2) in which the nature of the surface may be immediately appreciated. (See Davies, 1978, Chapter 11 for canonical reduction.) Figure 2 shows three other surface types representable by (3), the simple maximum, the saddle, and the stationary ridge. For additional details here, see Box, Hunter and Hunter (1978, pp. 526-534), the source from which Figures 1 and 2 were adapted.

The n sets of values $(x_{1u}, x_{2u}, \ldots, x_{ku})$ are the coded experimental design points, and may be regarded as a pattern of n points in a k-dimensional space. A response surface design is simply an experimental arrangement of points in x-space which permit the fitting of a response surface to the corresponding observations y_u. We thus speak of first order designs (if a



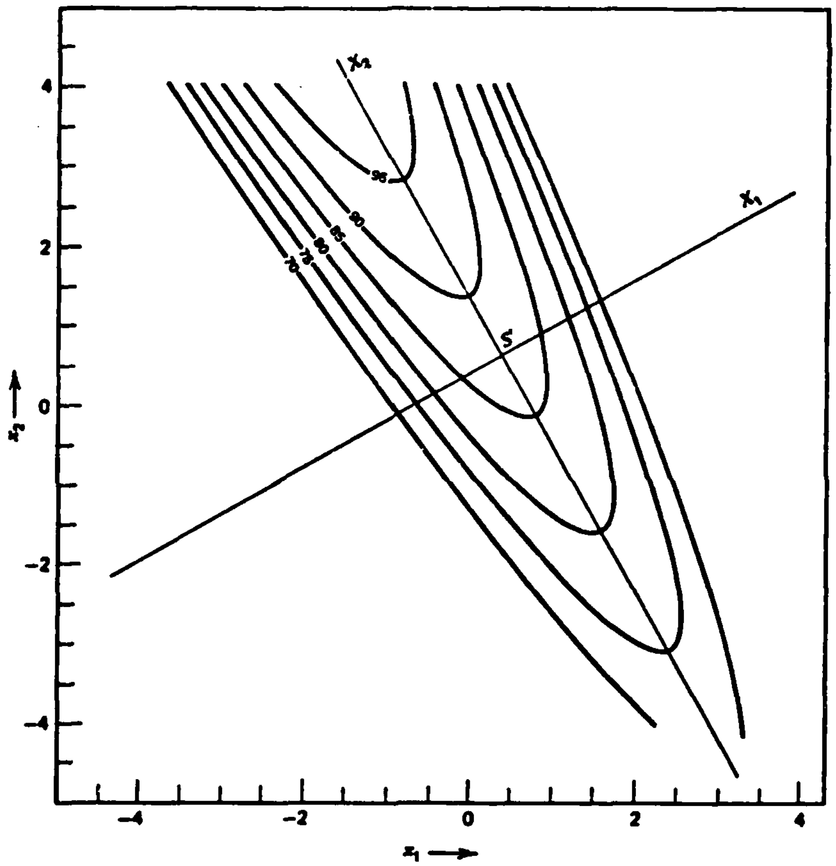


FIGURE 1 Example of a second-degree equation representing a rising ridge.

$$\hat{y} = 82.71 + 8.80x_1 + 8.19x_2 - 6.95x_1^2 - 2.07x_2^2 - 7.59x_1x_2$$
$$\hat{y} - 87.69 = -9.02X_1^2 + 2.97X_2$$

(a)

(b)

(c)

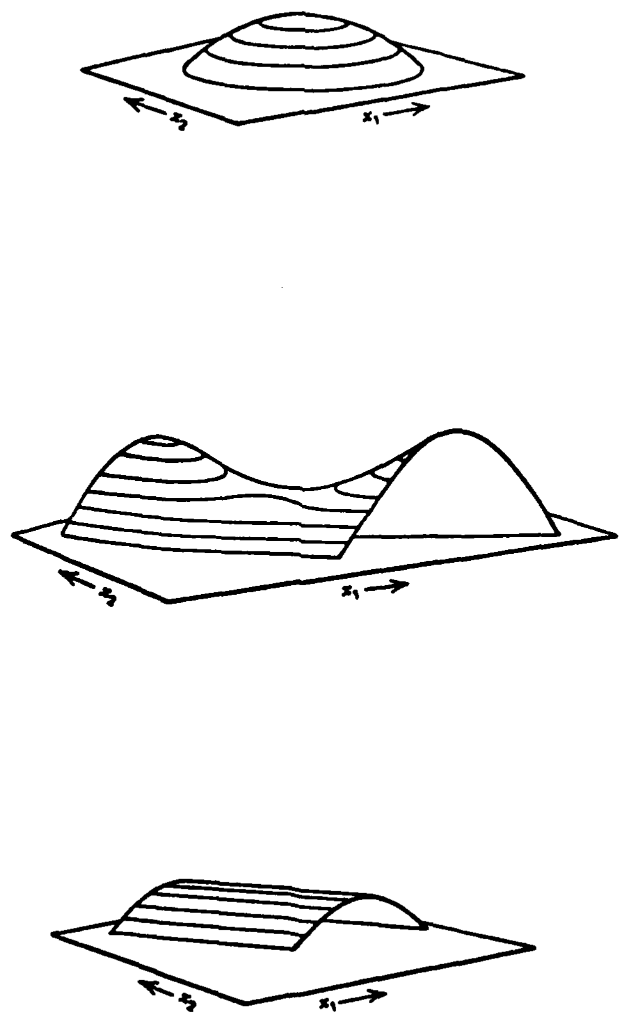


Figure 2. Examples of surfaces representable by a second-degree equation: (a) simple maximum, (b) saddle or col, (c) stationary ridge.

first order surface can be fitted), second order designs, and so on. Obviously, a design of a particular order is also necessarily a design of lower order.

The choice of a response surface design is thus one of selecting a set of suitable points in k-dimensional x-space according to some pre-selected criterion or criteria of goodness. The technical literature of experimental design contains many discussions of so-called "optimal designs". However, wary skepticism is called for in reading many of these papers, because their authors usually concentrate on one criterion only (and sometimes one that by practical experimental standards is inappropriate) and then derive the best designs under that single criterion. While this often provides interesting mathematical and/or computational exercises and throws light on the behaviour of the examined criterion, it does not necessarily lead to sound practical advice. There are many possible desirable characteristics for a "good" response surface design. Box and Draper (1975) gave fourteen such characteristics, any, all or some of which might in different circumstances be of importance. The design should:

1. generate a satisfactory distribution of information about the behaviour of the response variable throughout a region of interest, R;

2. ensure that the fitted value at x, $\hat{y}(x)$, be as close as possible to the true value at x, $\eta(x)$;

3. give good detectability of lack of fit;

4. allow transformations to be estimated;

5. allow experiments to be performed in blocks;

6. allow designs of increasing order to be built up sequentially;

7. provide an internal estimate of error;

8. be insensitive to wild observations and to violation of the usual normal theory assumptions;

9. require a minimum number of experimental points;

10. provide simple data patterns that allow ready visual appreciation;

11. ensure simplicity of calculation;

12. behave well when errors occur in the settings of the predictor variables, the x's;

13. not require an impractically large number of predictor variable levels;

14. provide a check on the 'constancy of variance' assumption.

Part of the art of the good practising statistician is his ability to assess the special needs of a given situation and to choose a design which comes close to meeting them. To aid this choice, it would be helpful, where possible, to have appropriate numerical measures of a design's desirability in relation to the various criteria. It would also be helpful to know which criteria are in conflict, and which in harmony. Much work remains to be done along these lines.

No design satisfies all the criteria simultaneously. However, there are types of designs which do satisfy many of them. Before discussing any particular designs we briefly elaborate on some of the features mentioned, using the same numbering.

1. In order that $\hat{y}(x)$ should be estimable for all x belonging to R, the main requirements are

(a) there must be enough design points to estimate all the coefficients, and preferably additional runs* to cover points 3 and 7.

(b) the number of levels of each x_i must exceed the order of the model; otherwise the $\underset{\sim}{X}'\underset{\sim}{X}$ matrix used in the least squares procedure will be singular.

6. It is an advantage if the observations used to fit, say, a first order model can be combined with some additional observations and re-used to fit a second order model, especially if a blocking scheme (see point 5) can be arranged so that differences in levels between the various blocks of the complete design do not affect the final estimates. Such an arrangement allows very economical use of experimental facilities. A design which can be built up in this way is called a sequentially blocked response surface design. Randomization of run order would be made only within blocks of the design.

7. The provision of an internal estimate of variance error can be achieved by using repeat (replicated) design points. These would often be repeats at the center of the design but, where the allowable number of runs permits it, non-central points could also be replicated. This latter course might be advisable if (i) it were known that the magnitudes of the errors were fairly large in relation to the average size of the observations to be used, and/or (ii) it was desired to measure the error variance at a number of $\underset{\sim}{x}$-locations (see 14), and/or (iii) some non-central region were of special interest.

A General Philosophy of Sequential Experimentation

The center of the experimental design is usually the point representing current "best" (whatever that is defined to mean) conditions, and the objective in empirically fitting a response surface may be

1. To examine the local nature of the relationship of the response and the predictors and so "explain" the response's behavior. It may, for example,

be desired to keep the response within specifications requested by a customer, and/or to see if predictor variable settings are critical and sensitive.

2. To proceed from the current "best" conditions to better conditions (lower cost, higher yield, improved tear resistance, and so on).

3. To use the fitted surface as a stepping stone to mechanistic understanding of the underlying process.

A more detailed list of possible objectives is given by Herzberg (1982).

We would usually first consider the possibility that a first order model might be satisfactory and perform a first order design. A simple but good choice (see Box, 1952) would be a simplex design with one or more center points. The general simplex in k dimensions has $n = k + 1$ points (runs) and can be oriented to have its coordinates given as in Table 1, where $a_i = \{cn/[i(i + 1)]\}^{1/2}$, and c is a scaling constant to be selected. Alternatively, a two-level factorial or fractional factorial, or a Plackett and Burman design*, with added center point(s) would be excellent. In all cases, the center point(s) average response can be compared to the average response at the non-central points to give a measure of non-planarity. For additional details, see Box, Hunter and Hunter (1978, p. 516).

x_1	x_2	x_3	...	x_i	...	x_k
$-a_1$	$-a_2$	$-a_3$	...	$-a_i$	...	$-a_k$
a_1	$-a_2$	$-a_3$	...	$-a_i$	...	$-a_k$
0	$2a_2$	$-a_3$	...	$-a_i$	...	$-a_k$
0	0	$3a_3$	...	$-a_i$	...	$-a_k$
.	.			.		.
.	.			.		.
.	.			.		.
				ia_i		
				0		
				.		
				.		
				.		
0	0	0		0		ka_k

Table 1. The Rows are the Coordinates of the $(k + 1)$ Points of a Simplex Design in k Dimensions.

If the first order surface fitted well, one would either interpret its nature if the local relationship were being sought, or else move out along a path of steepest ascent* (or descent) if improved conditions were sought; see Box, Hunter and Hunter (1978, p. 517). If the first order surface were an inadequate representation of the local data, either initially or after one or more steepest ascent(s) (or descent(s)), it would be sensible to consider transformations of the response and/or predictor variables which <u>would</u> allow a first order representation. When the possibilities of using first order surfaces had been exhausted, one would then consider a second order surface.

It would usually not be necessary at this stage to start from scratch, particularly if a two-level factorial* or fractional factorial* had just been used. This previous design could be incorporated as an orthogonal block in a larger second order composite design. We first explain how such a design is formed and then how orthogonal blocking may be achieved.

The Central Composite Design

A particular type of second order design which has many of the desirable features listed is the central composite design (normally called just the composite design). It is constructed from three sets of points. In the coded $\underset{\sim}{x}$-space, these three sets can be characterized as follows:

(a) the 2^k vertices $(\pm1,\pm1,\ldots,\pm1)$ of a k-dimensional "cube" $(k < 4)$, or a fraction of it $(k > 5)$,

(b) the $2k$ vertices $(\pm\alpha,0,\ldots,0)$, $(0,\pm\alpha,\ldots,0),\ldots,(0,0,\ldots,0,\pm\alpha)$ of a k-dimensional cross-polytope or "star",

(c) a number, n_0, of "center points", $(0,0,\ldots,0)$.

Set (a) is simply a full 2^k factorial design or a 2^{k-p} fractional factorial if $k > 5$. The notation $(\pm1,\pm1,\ldots,\pm1)$ means that 2^k points obtained by taking all possible combinations of signs are used for full factorial cases. (In response surface applications, these points are often referred to as a "cube", whatever the number of factors may be.)

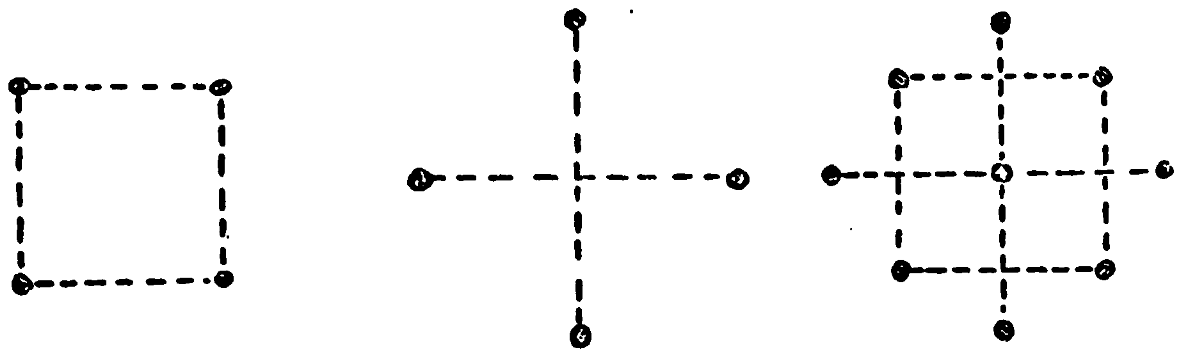
Set (b) consists of pairs of points on the coordinate axes all at a distance α from the origin. (The quantity α has yet to be specified; according to its value the points may lie inside or outside the cube.) In three dimensions the points are the vertices of an octahedron and this word is sometimes used for other values of $k \neq 3$. However, a more convenient name for such a set of points in k dimensions is "star" or, more formally, cross-polytope.

These sets and the complete design (the n_0 center points represented by a single center point) are shown diagrammatically in Figures 3 and 4 for the cases $k = 2$ and 3.

Fractionation of the cube is possible whenever the resulting design will permit individual estimation of all the coefficients in Eq. (3). For this, the fraction must have resolution greater than or equal to five. (See article on Plackett and Burman designs and references therein for resolution.) The smallest usable fraction is then a 2^{k-1} design (a half-fraction) for $k = 5,6,7$, a 2^{k-2} design (a quarter fraction) for $k = 8,9$, a 2^{k-3} for $k = 10$, and so on. (See Box, Hunter, and Hunter, 1978, p. 408.) Table 2, adapted from Box and Hunter (1957, p. 227) shows the number of parameters in Eq. (3) and the number of non-central design points in the corresponding composite design for $k = 2,\ldots,9$. The values to be substituted for p are $p = 0$ for $k = 2,3,$ and 4; $p = 1$ for $k = 5,6$ and 7; and $p = 2$ for $k = 8$ and 9; they correspond to the fraction, $1/2^p$, of the cube used for the design.

No. of variables	k	2	3	4	5	6	7	8	9
No. of parameters	$(k+1)(k+2)/2$	6	10	15	21	28	36	45	55
Cube + star	$2^k + 2k$	8	14	24	-	-	-	-	-
$\frac{1}{2}$(Cube) + star	$2^{k-1} + 2k$	-	-	-	26	44	78	-	-
$\frac{1}{4}$(Cube) + star	$2^{k-2} + 2k$	-	-	-	-	-	-	80	130
α (rotatable)	$2^{(k-p)/4}$	1.414	1.682	2	2	2.378	2.828	2.828	3.364
Suggested n_0		2-4	2-4	2-4	0-4	0-4	2-4	2-4	2-4

Table 2. Features of Certain Composite Designs.

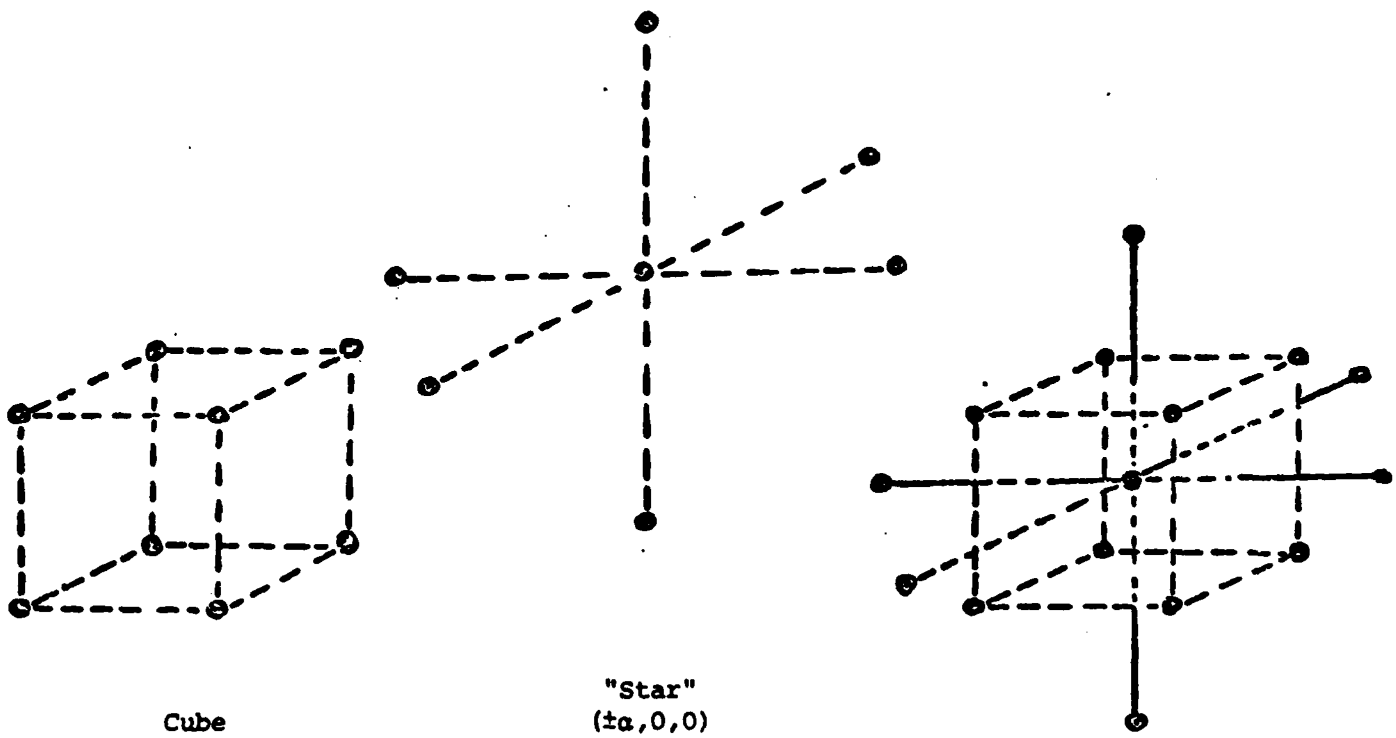


"Cube" ($\pm 1, \pm 1$)

"Star" ($\pm\alpha$,0) (0,$\pm\alpha$)

"Cube" + "Star" + Center points

Figure 3. Composite design for $k = 2$ variables.



Cube ($\pm 1, \pm 1, \pm 1$)

"Star" ($\pm\alpha$,0,0) (0,$\pm\alpha$,0) (0,0,$\pm\alpha$)

Cube + "Star" + Center points

Figure 4. Composite design for $k = 3$ variables.

We can check immediately that the composite designs have at least some of the 14 desirable features. For example, there are enough points and enough levels (three if $\alpha = 1$, five if $\alpha \neq 1$) to satisfy points 1 and 13. The designs can be performed sequentially; the cube or factorial portion plus center points can be used as a first order design and the additional star points, plus center points complete the second order design. Thus points 5 and 6 are achieved. (If a block effect changes the response level between the running of the two sections, it will usually be detected through the center point readings. The block effect could be estimated as the difference between the average responses at the center levels in each of the two blocks and the observations in one or the other block could be appropriately adjusted, if desired. Alternatively, the design can be orthogonally blocked, that is, blocked in such a way that block effects are orthogonal to model estimates and so do not affect them; see below.)

The n_0 repeated center points allow the internal (pure error) estimation of error as in point 7. The number of design points is reasonable in relation to the number of coefficients if not minimal (point 9). The pattern of the design (point 10) is clearly excellent, and the least squares calculations are simple (point 11). The designs are also robust to small errors in the settings of the x's since a slight displacement of the design points will not materially affect the fitted surface (point 12). However, a wild observation may cause an erroneous displacement of the fitted surface (point 8). This can often be detected from the patterns exhibited by the standard residuals plots if the effect is serious. The size of a possible displacement may be reduced if all or some of the noncentral design points are replicated, since in a set of repeats a single wild observation will be "muted" by its "correct" replicates. Points 2 and 3 can be satisfied by choice of α, n_0, and by shrinking or expanding all the design points relative to the region R (see Box and Draper, 1959, 1963). See, also, Welch (1983) and Houck and Myers (1978). Point 4 is also satisfied (see Box and Draper, 1982). Overall then, the composite design is an excellent choice.

What values should be chosen for α and n_0? The value of α determines if the star points fall inside the cube $(\alpha < 1)$, outside the cube $(\alpha > 1)$, or on the faces of the cube $(\alpha = 1)$. Note that when $\alpha = 1$ only three experimental levels $(-1,0,1)$ are required, which may be an advantage or necessity in some experimental situations. For additional comments and specific designs see De Baun (1959) and Box and Behnken (1960).

If three levels are not essential, what value of α should be selected? One criterion that can be applied to decide this is that of <u>rotatability</u>*. A design (of any order) is rotatable when the contours of the variance function $V\{\hat{y}(x)\}$ are spheres about the origin in the k-dimensional factor space defined by variables $x_1, x_2, \ldots, x_k$. Box and Hunter (1957) showed that the required values (given in Table 2) are $\alpha = 2^{(k-p)/4}$, where $p = 0$, 1 or 2 according to the fraction of the cube used in the design.

Note that the rotatability property is specifically related to the codings chosen for the x's. It is usually assumed that the experimenter has chosen these codings in such a manner that she anticipates (roughly speaking) that one unit of change in any x will have about the same effect on the response variable. In such a case, obtaining equal information at the same radial distance in any direction (which is what rotatability implies) is clearly sensible. Codings are rarely perfect; the experimenter adjusts the codings in future designs as a result of information gained in current and past experiments. Exact rotatability is not a primary consideration.

However, knowledge of the tabulated values provides a target to aim at, while one is attempting to satisfy other desirable design features.

How large a value should be selected for n_0? There are many possible criteria to apply; these are summarized by Draper (1982, 1984). The suggested values in the table are ones that appear to be sensible with respect to many criteria, the overall message being that only a few center points are usually needed. (Whenever α is chosen so that all the design points lie on a sphere, at least one center point is essential, otherwise not all of the coefficients can be individually estimated.) A few additional center points will do no harm. Nevertheless, additional runs are probably better used to duplicate selected non-central design points, unless special considerations apply, as below. Repeated points spread over the design provide a check of the usual "homogeneous variance" assumption; see Box (1959) and Dykstra (1960).

For a numerical example of a second order response surface fitting for $k = 3$, see Draper and Smith (1981, pp. 390-403).

Orthogonal Blocking

Another criterion (previously mentioned) that may be applied to the choice of α and n_0 in the composite design is that of <u>orthogonal blocking</u>. This requires division of the runs into two or more blocks in such a manner that this division does not affect the estimates of the second order model obtained via the standard least squares regression analysis. The basic approach was given by Box and Hunter (1957); see, also, DeBaun (1956) and Box (1959). Two conditions must be satisfied:

1. Each block must itself be a first order orthogonal design. Thus $\sum_u x_{iu}x_{ju} = 0$, $i \neq j$, for each block.

2. The fraction of the total sum of squares of each variable x_i contributed by every block must be equal to the fraction of the total observations allotted to the block. Thus, for each block,

$$\frac{\sum_u x_{iu}^2}{\sum_{u=1}^{n} x_{iu}^2} = \frac{n_b}{n} \tag{4}$$

where n_b denotes the number of runs in the block under consideration, $\sum_u$ denotes summation only in that block, and the denominators of (4) refer to the entire design.

The simplest orthogonal block division of the composite design is into the orthogonal design pieces:

Block 1. Cube portion (2^{k-p} points) plus c_0 center points.

Block 2. Star portion ($2k$ points) plus s_0 center points.

Application of (4) then implies that

$$\alpha = \{2^{k-p-1}(2k + s_0)/(2^{k-p} + c_0)\}^{1/2}. \tag{5}$$

For example, if $k = 3$, $p = 0$, so that the first block is a 2^3 factorial plus c_0 center points and the second block is a six point octahedron plus s_0 center points, then

$$\alpha = \{4(6 + s_0)/(8 + c_0)\}^{1/2}. \tag{6}$$

If $c_0 = 4$ center points are added to the cube and no center points are added to the star ($s_0 = 0$), then $\alpha = 2^{1/2} = 1.414$. This design is orthogonally blocked but is not rotatable. However, values of α closer to the rotatable value 1.682 are possible. For example, if $c_0 = 0$, $s_0 = 0$, $\alpha = (24/8)^{1/2} = 1.732$; or if $c_0 = 4$, $s_0 = 2$, $\alpha = (32/12)^{1/2} = 1.633$. The choices are, of course, limited by the fact that c_0 and s_0 must be integers. Generally, orthogonal blocking (α from (6)) takes precedence over rotatability, for which $\alpha = 2^{(k-p)/4}$ is needed. In certain cases, both can be achieved simultaneously. This requires

$$2^{k-p} + c_0 = 2^{\frac{1}{2}(k-p)-1}(2k + s_0) \tag{7}$$

to be satisfied for integer (k,p,c_0,s_0). Some possibilities are $(2,0,s_0,s_0)$, $s_0 \geq 1$, $(4,0,2s_0,s_0)$, $(5,1,(4 + 2s_0),s_0)$, $(7,1,4(s_0 - 2),s_0)$, $s_0 \geq 2$, $(8,2,4s_0,s_0)$, where $s_0 = 0,1,2,\ldots,$ unless otherwise specified. (Note that some of these arrangements call for more center points than recommended in the table, an example of how applications of different criteria can produce conflicting conclusions.)

Further division of the star will not lead to an orthogonally blocked design. However, it is possible to divide the cube portion into smaller blocks and still maintain orthogonal blocking if $k > 2$. As long as the pieces which result are fractional factorials of resolution III or more (see Box, Hunter and Hunter, 1978, p. 385), each piece will be an orthogonal design. All fractional factorial pieces must contain the same number of center points or else (4) cannot be satisfied. Thus c_0 must be divisible by the number of blocks.

An Attractive Three-Factor Design

In a composite design, replication of either the cube portion or the star portion, or both can be chosen if desired. As an example of such possibilities, we now provide, in Table 3, a 24 run second order design for three factors which is rotatable and orthogonally blocked into four blocks of equal size. It consists of a cube (fractionated via $x_1x_2x_3 = \pm 1$) plus replicated (doubled) star plus four center points, two in each 2^{3-1} block. This design provides an illustration of the fact that center points in different blocks of the design are no longer comparable due to possible block effects. Thus, the sum of squares for pure error must be obtained by pooling the separate sums of squares for pure error from each block.

	x_1	x_2	x_3	
	-1	-1	1	
	1	-1	-1	2^{3-1} design,
	-1	1	-1	$x_1x_2x_3 = 1$
Block I	1	1	1	plus two
	0	0	0	center points
	0	0	0	
	-1	-1	-1	
	1	-1	1	2^{3-1} design,
	-1	1	1	$x_1x_2x_3 = -1$
Block II	1	1	-1	plus two
	0	0	0	center points
	0	0	0	
	$-2^{1/2}$	0	0	
	$2^{1/2}$	0	0	
Block III	0	$-2^{1/2}$	0	star,
	0	$2^{1/2}$	0	$\alpha = 2^{1/2}$
	0	0	$-2^{1/2}$	
	0	0	$2^{1/2}$	
	$-2^{1/2}$	0	0	
	$2^{1/2}$	0	0	
Block IV	0	$-2^{1/2}$	0	star,
	0	$2^{1/2}$	0	$\alpha = 2^{1/2}$
	0	0	$-2^{1/2}$	
	0	0	$2^{1/2}$	

Table 3. A 24 Run Second Order Rotatable Response Surface Design for Three Factors, Orthogonally Blocked into Four Blocks of Equal Size.

General Comment

A second order response surface design will be very effective if the underlying surface being examined is roughly quadratic. If it is an attenuated or distorted quadratic, transformations on the x-variables will often be needed. In practice, one usually discovers the need for such transformations by observing the non-quadratic curvature in the data after a second order design has been used and finding that the fitted quadratic surface cannot properly handle that curvature.

Qualitative Variables

Our discussion so far has effectively assumed that all the ξ's are quantitative variables able to assume any value in some specified range limited only by the practicalities of the experimental situation. In some experimentation, some of the predictor variables are qualitative, that is, able to take only distinct values. For example, three different catalysts might constitute three qualitative levels of one factor. So might three fertilizers, unless they were constructed, for example, by altering the level of an ingredient; in such a case, the three fertilizers would usually be regarded as constituting three levels of a continuous variable. Variables such as shifts, reactors, operators, machines, and railcars would, typically, be qualitative variables. When qualitative variables occur in a response surface study, surfaces in the quantitive variables are fitted separately for each combination of qualitative variables. For illustrative commentary see Box, Hunter and Hunter (1978, pp. 296-299).

Analysis for Orthogonally Blocked Designs

When a second order design is orthogonally blocked:

1. Estimate the β-coefficients of the second order model in the usual way, ignoring blocking.

2. Calculate pure error from repeated points <u>within</u> the same block only, and then combine these contributions in the usual way. Runs in different blocks cannot be considered as repeats.

3. Place an extra term

$$SS(\text{blocks}) = \sum_{w=1}^{m} \frac{B_w^2}{n_w} - \frac{G^2}{n},$$

with $(m - 1)$ degrees of freedom in the analysis of variance table, where B_w is the total of the n_w observations in the w-th block and G is the grand total of all the observations in all the m blocks.

Further Reading

The literature of response surface methodology is very extensive. For readers who would like to know more, about response surface methodology, we encourage the following course of action.

1. Obtain an overview of the field from the excellent review papers of Mead and Pike (1975) and Morton (1983). (Although the former paper is "from a biometric viewpoint", it will also serve the non-biometric viewpoint reader extremely well.) Then look at the earlier review papers of Hill and Hunter (1966) and Herzberg and Cox (1969) for additional broadening.

2. Read the succession of key papers by Box and Wilson (1951), Box (1952), Box (1954), Box and Youle (1955), and Box and Hunter (1957). They contain the basic ideas and philosophy essential to a full understanding of

the field. (Although the fundamental ideas of response surface methodology (RSM) existed before his series of contributions began, George E. P. Box is justifiably regarded as the founding father of modern RSM. His succession of publications, written alone and with co-authors, extends over several decades.)

3. For a definitive textbook account of response surface methodology, see Box and Draper (1985?). Less extensive accounts may also be found in other texts, for example, Box, Hunter and Hunter (1978), Davies (1978), Guttman, Wilks and Hunter (1971) and Myers (1971). For response surface applications in experiments with mixtures of ingredients, see Cornell (1981).

4. Readers interested in the mathematical and computational problems of "optimal design" theory with its various alphabetic optimality criteria should read the ingenious contributions of J. Kiefer, his co-authors, and others. For references see, for example, St. John and Draper (1975), Herzberg (1982), and Kiefer (1984). For a discussion of the problems, see Box (1982), summarized in Box and Draper (1985?, Chapter 14). See also Lucas (1976) and Atkinson (1982). For the application of optimality criteria for compromise purposes, for example, to obtain designs which can be reasonably efficient both for model testing and parameter estimation, see Atkinson (1975).

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The fitting of first and second degree equations to experimental data in order to summarize the main features of the underlying but unknown mechanism, is a useful and widely used technique. In addition to its interpretive value, it often provides information about the mechanism. Certain ways of obtaining the data are better than others. Criteria for choice of a suitable response surface

20. ABSTRACT - Cont'd.

design, and specific designs that have excellent characteristics with respect to those criteria, are described in this expository article. Various other related features, suggestions for further reading, and a list of basic references are included.

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