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Report No. 23

IDENTIFICATION OF ACTIVE FACTORS IN UNREPLICATED FRACTIONAL FACTORIAL EXPERIMENTS

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February 1987

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PRACTICAL SIGNIFICANCE

Fractional factorial experiments are used to simultaneously assess the effects and interactions of many factors affecting a product or process. One drawback in this approach is that the small number of runs per factor means there are several explanations for the experimental data, and it can be difficult to associate the observed results with a particular factor or combination of factors. But with proper analysis, the number of possible explanations can be reduced at each round of experimentation, the most likely explanation still identified in fewer total runs than in a full factorial experiment. The information needed to separate likely and unlikely explanations comes from prior knowledge of the system as well as experimental data. A good statistical analysis will not only use both sources, it will also take the uncertainty of the information into account. This report examines these issues and explores how sensitive the analysis is to various assumptions typically made about the factors and data.

Key Words: Fractional factorial; unreplicated; factor sparsity; posterior probability.

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1. Introduction

A recent article by Box and Meyer (1986) describes an analysis for unreplicated fractional factorials motivated by the hypothesis of factor sparsity. A condition of factor sparsity is said to exist when only a small proportion of the experimental factors have large effects relative to noise. A two-stage approach is typically used for analyzing unreplicated factorials under such conditions. At the first stage of the analysis we attempt to identify those contrasts that are too large to be explained by noise: these may be called active contrasts. A graphical method for doing this involves plotting the contrasts on normal probability paper (Daniel, 1959). Box and Meyer (1986) describe a more formal analysis in which the posterior probability that a contrast is active is computed. The posterior probabilities can be displayed graphically to provide a useful supplement to the normal plot. The second stage of the two-stage approach would involve associating the supposed active contrasts with specific factors, either as main effects or interactions.

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Box and Hunter (1961) offered two guidelines for the process of matching factorial effects with active contrasts in the presence of the confounding usually associated with fractional factorials:

1. Main effects are more likely to occur than two-factor interactions, which are more likely than three-factor interactions, etc. That is, if a large contrast is associated with more than one effect, the effect of lowest order is usually considered the most likely cause. This is especially true for continuous variables, when smoothness of the response surface dictates that higher-order effects, which correspond to higher-order derivatives, become successively smaller. In screening situations and other applications, it is common to ignore three-factor or higher-order interactions.
2. Variables that have large main effects are more likely to have significant interactions among themselves or with other variables. For example, when a large contrast is associated with several two-factor interactions, the interactions involving variables with large main effects are considered more likely to be the explanation.

Box and Hunter emphasized that these guidelines were to be employed to make tentative conclusions, subject to verification by subsequent experimentation or monitoring of a process after implementing changes. Exceptions to the rules appear, for example, when the design is located on a diagonal ridge of the response surface. This can occur when a process has been fine-tuned in the past one variable at a time, in the presence of compensating factors, such as time and temperature of a chemical reaction. The experiment will then produce small main effects among the compensating factors, but a large two-factor interaction.

Temporary assumptions used in the first stage of the analysis, and incorporated into the normal plot and computing of posterior probabilities, are that each of the observed contrasts is equally likely to be active, that contrasts are active independent of one another, and that active contrasts are expected to be the same size whether they are main effects or interactions. These assumptions are dropped at the second stage of the analysis in favor of those given by Box and Hunter (1961). (The constant reinterpretation of results by withdrawing assumptions made at a previous step is a vital component of statistical analysis. See Box, 1980.) The purpose of this article is to explore the application of Box and Meyer's (1986) analysis to the second stage, or, alternatively, to incorporate the second-stage assumptions into the computation of posterior probabilities.

2. Model Assumptions

It is assumed that the design matrix $\underset{\sim}{X}$ is a $n \times n$ orthogonal matrix of ± 1s such that $\underset{\sim}{X}'\underset{\sim}{X} = \underset{\sim}{X}\underset{\sim}{X}' = n\underset{\sim}{I}_n$, where $\underset{\sim}{I}_n$ is the $n \times n$ identity matrix. The first column $\underset{\sim}{x}_0$ of $\underset{\sim}{X}$ is a column of 1s, and some or all of the remaining columns $\underset{\sim}{x}_1, \ldots, \underset{\sim}{x}_{n-1}$ are assigned to experimental variables; -1 denoting the low or nominal level and $+1$ denoting the high or alternate level. At the completion of the experiment the $n \times 1$ vector $\underset{\sim}{y} = (y_1, \ldots, y_n)'$ becomes available, and the orthogonal contrasts $T_i = \underset{\sim}{x}_i'\underset{\sim}{y}/n$, $i = 1, \ldots, n-1$, are computed, $\underset{\sim}{T} = (T_1, \ldots, T_{n-1})'$.

A general framework for the approach of Box and Meyer (1986) is now described. Let $a_{(r)}$ denote the event that a particular combination of r of the $n - 1$ contrasts are active, the remainder inert. (There are $\binom{n-1}{r}$ different events $a_{(r)}$, but the generic notation $a_{(r)}$ is used for convenience to refer to a particular one of these.) Let $\underset{\sim}{X}_{(r)}$ refer to the $n \times (r+1)$ matrix of columns of $\underset{\sim}{X}$ corresponding to the active contrasts of $a_{(r)}$, and let $\underset{\sim}{\tau}_{(r)}$ be the $(r+1) \times 1$ vector of true effects (regression coefficients) under $a_{(r)}$. ($\underset{\sim}{X}_{(r)}$ and $\underset{\sim}{\tau}_{(r)}$ include an extra column $\underset{\sim}{x}_0$ and component τ_0, respectively, for the overall mean.) The sampling distribution of the vector of observations $\underset{\sim}{y}$, given $a_{(r)}$, is

$$p(\underset{\sim}{y}|a_{(r)}, \underset{\sim}{\tau}_{(r)}, \sigma^2) \propto \sigma^{-n} \exp\left\{-\frac{1}{2\sigma^2}(\underset{\sim}{y} - \underset{\sim}{X}_{(r)}\underset{\sim}{\tau}_{(r)})'(\underset{\sim}{y} - \underset{\sim}{X}_{(r)}\underset{\sim}{\tau}_{(r)})\right\} . \qquad (1)$$

Suppose further that the prior distributions of the elements of $\underset{\sim}{\tau}_{(r)}$, except τ_0, are independent and normal with zero mean and variance $\gamma^2\sigma^2$, with noninformative priors for τ_0 and σ (see Box and Tiao, 1973), so that

$$p(\underset{\sim}{\tau}_{(r)}|a_{(r)}, \sigma) \propto (\gamma\sigma)^{-r} \exp\left\{-\frac{1}{2\sigma^2}\underset{\sim}{\tau}_{(r)}'\underset{\sim}{\Gamma}_r\underset{\sim}{\tau}_{(r)}\right\}$$

$$p(\sigma) \propto \frac{1}{\sigma} \qquad (2)$$

where the $(r+1) \times (r+1)$ matrix

$$\Gamma_r = \frac{1}{\gamma^2}\begin{bmatrix} 0 & 0' \\ 0 & I_r \end{bmatrix}$$

and I_r is the $r \times r$ identity matrix.

To model the assumption that a majority of the contrasts are expected to be inert, let α be the prior probability that any particular contrast is active. The prior probability of the event $a_{(r)}$ is $p(a_{(r)}) = \alpha^r(1-\alpha)^{n-r-1}$, assuming contrasts are active independent of one another. After observing data y from the experiment, a general formula for the posterior probability of the event $a_{(r)}$ is

$$p(a_{(r)}|y) = \frac{p(y|a_{(r)})p(a_{(r)})}{\sum_{(i)} p(y|a_{(i)})p(a_{(i)})} \tag{3}$$

where the denominator is the summation over all possible combinations of active and inert contrasts, and $p(y|a_{(r)})$ is the predictive density of y given $a_{(r)}$,

$$p(y|a_{(r)}) = \int p(y|a_{(r)},\tau_{(r)},\sigma)p(\tau_{(r)}|a_{(r)},\sigma)p(\sigma)d\tau_{(r)}d\sigma \; . \tag{4}$$

In particular, the probability $p(a_{(r)}|y)$ is

$$p(a_{(r)}|y) \propto \left(\frac{\alpha}{1-\alpha}\right)^r \gamma^{-r} \frac{|X'_{(0)}X_{(0)}|^{1/2}}{|\Gamma_r + X'_{(r)}X_{(r)}|^{1/2}} \times$$

$$\left[\frac{S(\hat{\tau}_{(r)}) + \hat{\tau}'_{(r)}\,\Gamma_r\,\hat{\tau}_{(r)}}{S(\hat{\tau}_{(0)})}\right]^{-\frac{(n-1)}{2}} \tag{5}$$

where

$$\hat{\tau}_{(r)} = (\Gamma_r + X'_{(r)}X_{(r)})^{-1}X'_{(r)}y$$

and

$$S(\hat{\tau}_{(r)}) = (y - X_{(r)}\hat{\tau}_{(r)})'(y - X_{(r)}\hat{\tau}_{(r)}) \; .$$

For the orthogonal design $\underset{\sim}{X}$ defined earlier this reduces further to

$$p(a_{(r)}|\underset{\sim}{y}) \propto \left(\frac{\alpha}{1-\alpha}\right)^{r} k^{-r} \left| 1 - \varphi \frac{\underset{\sim}{T}'_{(r)}\underset{\sim}{T}_{(r)}}{\underset{\sim}{T}'\underset{\sim}{T}} \right|^{-(n-1)/2} \tag{6}$$

where $k^2 = n\gamma^2 + 1$, $\varphi = 1 - 1/k^2$, $\underset{\sim}{T}_{(r)}$ is the vector of r observed contrasts corresponding to $a_{(r)}$, and $\underset{\sim}{T}$ is the complete vector of $n - 1$ contrasts. Box and Meyer (1986) showed how the parameter k^2 represents the ratio of the average squared active contrast over the average squared inert contrast. The probabilities $p(a_{(r)}|\underset{\sim}{y})$ can be summed to give the posterior probability that a particular contrast is active,

$$p_i = P[\text{contrast } T_i \text{ active} \mid \underset{\sim}{y}] = \sum_{(r):i \text{ active}} p(a_{(r)}|\underset{\sim}{y}) \ . \tag{7}$$

The temporary assumptions of stage one described in Section 1 correspond to

(i) the $n - 1$ contrasts have equal prior probability α of being active,

(ii) contrasts are active independently,

(iii) the prior parameter k (or γ) is the same for each effect τ_i.

Modifications to the model introduced above are now given to incorporate the stage-two assumptions. It is assumed that factors will be active in producing main effects and interactions with prior probability α. In general this value of α will be different from the value used to describe the frequency of active contrasts. Let $a_{(f)}$ be the event that a particular combination of f factors is active. Let $\underset{\sim}{X}_{(f)}$ be the matrix of columns corresponding to the active effects of $a_{(f)}$ (including interaction columns and a column for the overall mean.) For example, if $a_{(f)}$ is the event that factors 1 and 2 are active, $\underset{\sim}{X}_{(f)}$ would contain columns for the main effects of factors 1 and 2, as well as a cross-product column for the associated two-factor interaction. Likewise let $\underset{\sim}{\tau}_{(f)}$ be the vector of true effects under $a_{(f)}$.

The sampling distribution of the vector of observations $\underset{\sim}{y}$, given $a_{(f)}$, is

$$p(\underset{\sim}{y}|a_{(f)},\sigma,\underset{\sim}{T}_{(f)}) \propto \sigma^{-n}\exp\{\frac{-1}{2\sigma^2}(\underset{\sim}{y} - \underset{\sim}{X}_{(f)}\underset{\sim}{T}_{(f)})'(\underset{\sim}{y} - \underset{\sim}{X}_{(f)}\underset{\sim}{T}_{(f)})\} . \qquad (8)$$

The elements of $\underset{\sim}{T}_{(f)}$ are assumed to have independent, but not nece identical, prior normal distributions as before. In particular, it will be assumed that elements of $\underset{\sim}{T}_{(f)}$ which are main effects will have prior distributions with mean 0 and variance $\gamma_1^2\sigma^2$, and those elements which are two-factor interactions will have mean 0 and variance $\gamma_2^2\sigma^2$. And, though this assumption is not necessary, for ease of illustration it will be assumed that interactions between three or more factors are inert. A noninformative prior distribution is assumed again for the overall mean τ_0 and $\log(\sigma)$. The posterior probability of the event $a_{(f)}$ can then be written

$$p_{(f)} = p(a_{(f)}|y) \propto \left(\frac{\alpha}{1-\alpha}\right)^f \gamma_1^{-f}\gamma_2^{-f(f-1)/2} \times$$

$$\frac{|\underset{\sim}{X}_0'\underset{\sim}{X}_0|^{1/2}}{|\underset{\sim}{\Gamma}_f + \underset{\sim}{X}_{(f)}'\underset{\sim}{X}_{(f)}|^{1/2}} \left|\frac{S(\hat{\underset{\sim}{T}}_{(f)}) + (\hat{\underset{\sim}{T}}_{(f)}'\underset{\sim}{\Gamma}_f\hat{\underset{\sim}{T}}_{(f)})}{S(\hat{\underset{\sim}{T}}_{(0)})}\right|^{-(n-1)/2} , \qquad (9)$$

where

$$\hat{\underset{\sim}{T}}_{(f)} = [\underset{\sim}{\Gamma}_f + \underset{\sim}{X}_{(f)}'\underset{\sim}{X}_{(f)}]^{-1}\underset{\sim}{X}_{(f)}'\underset{\sim}{y} , \qquad (10)$$

$\underset{\sim}{\Gamma}_f$ is the diagonal matrix with the appropriate diagonal elements (the (1,1) element is zero, the (i,i) element is $1/\gamma_1^2$ if the ith element of $\underset{\sim}{T}_{(f)}$ is a main effect, $1/\gamma_2^2$ if an interaction), and $S(\hat{\underset{\sim}{T}}_{(f)})$ is the residual sum of squares obtained when estimating $\underset{\sim}{T}_{(f)}$ by $\hat{\underset{\sim}{T}}_{(f)}$. (Allowance for possible higher-order interactions can be made by appropriate redefinition of $\underset{\sim}{X}_{(f)}$ and $\underset{\sim}{T}_{(f)}$ and the exponent of γ_2, or introduction of a third parameter γ_3.) For a 2^{k-p} fractional factorial (Box and Hunter, 1961) $\underset{\sim}{X}_{(f)}$ is orthogonal and we can make the transformation

$$k_j^2 = n\gamma_j^2 + 1 ,$$

so that the probability $p_{(f)}$ can be rewritten, analogous to equation (6),

$$p_{(f)} \propto \left(\frac{\alpha}{1-\alpha}\right)^f k_1^{-f} k_2^{-f(f-1)/2} \times \left[1 - \varphi_1 \frac{\underset{\sim}{T}'_{m(f)}\underset{\sim}{T}_{m(f)}}{\underset{\sim}{T}'\underset{\sim}{T}} - \varphi_2 \frac{\underset{\sim}{T}'_{i(f)}\underset{\sim}{T}_{i(f)}}{\underset{\sim}{T}'\underset{\sim}{T}}\right]^{-(n-1)/2} , \tag{11}$$

where $\underset{\sim}{T}_{m(f)}$ is the vector of observed contrasts that are main effects under $a_{(f)}$, $\underset{\sim}{T}_{i(f)}$ is the vector of contrasts that are interactions under $a_{(f)}$, and $\varphi_j = 1 - 1/k_j^2$.

The probabilities $p_{(f)}$ can be accumulated to compute the marginal posterior probability p_j^* that factor j is active,

$$p_j^* = \sum_{(f):j \text{ active}} p_{(f)} . \tag{12}$$

Relaxing the Bound on f

For application to 2^{k-p} fractional factorials of resolution III and IV (Box and Hunter, 1961) the above definitions are consistent so long as f is restricted to be smaller than the design resolution.

The assumption that the number of active factors is less than the design resolution may be unreasonable for fractional factorial designs of low resolution. Suppose that eight factors were screened using a 2^{8-4} design of resolution IV. In this situation it is unknown which of eight factors is important, and although the experimenter supposes that at most three are active, it is possible that more than three are active. A natural extension of the above ideas to allow relaxation of the bound on f is given for the 2^{k-p} designs.

Consider a combination of f factors denoted by $a_{(f)}$, where f is greater than or equal to the design resolution R. Suppose there is confounding among the possible main effects and interactions of $a_{(f)}$, i.e., there are column contrasts which estimate more than one of the possible effects under $a_{(f)}$. (It is possible to have combinations of f factors with $f > R$ for which there is no confounding, and no modification is necessary for these.) For those columns which estimate more than one effect, define the corresponding element of $\underset{\sim}{\tau}_{(f)}$ to be the linear combination of effects estimated by that column contrast. The prior distributions for such elements of $\underset{\sim}{\tau}_{(f)}$ will still be independent and normal, but with variance equal to the sum of the variances for the individual components. For example, if a particular column contrast T_i estimated the sum of two two-factor interactions, the prior variance of τ_i would be $2\gamma_2^2\sigma^2$. All further computations proceed as usual given this modification of the prior distribution of $\underset{\sim}{\tau}_{(f)}$. For example, consider a combination of four factors which are confounded from the 2^{8-4} design of resolution IV. (The product of the columns of any three of the factors gives the column of the remaining factor.) There will be three column contrasts each of which estimates the sum of two two-factor interactions among the four factors. The posterior probability of this combination is given by (assuming interactions between three or more factors to be inert)

$$p_{(f)} \alpha \left(\frac{\alpha}{1-\alpha}\right)^4 k_1^{-4} (2^{1/2} k_2)^{-3} \times$$

$$\left| 1 - \varphi_1 \frac{\underset{\sim}{T}'_{m(f)} \underset{\sim}{T}_{m(f)}}{\underset{\sim}{T}'\underset{\sim}{T}} - \varphi_2 \frac{\underset{\sim}{T}'_{i(f)} \underset{\sim}{T}_{i(f)}}{\underset{\sim}{T}'\underset{\sim}{T}} \right|^{-(n-1)/2} , \qquad (13)$$

where $\underset{\sim}{T}_{i(f)}$ is the vector of three contrasts each estimating a sum of two interactions. The expression for $p(a_{(f)}|\underset{\sim}{y})$ can now be computed for any f without numerical difficulties.

Plackett and Burman Designs

For the orthogonal two-level designs of Plackett and Burman (1946) which are not 2^{k-p} designs, the simplification of equation (11) does not hold. The matrix $\underset{\sim}{X}_{(f)}$ of linear and cross-product columns for such designs is not orthogonal in general, and the cross product columns are not columns in the original design matrix $\underset{\sim}{X}$. However, as long as f is small enough, the matrix $\underset{\sim}{X}_{(f)}$ will be nonsingular and equation (9) can be used to compute $p(a_{(f)}|\underset{\sim}{y})$. For example, the bound on f for an arbitrary assignment of columns to the 12-run Plackett-Burman design is 4.

3. Initial Parameters

The parameters α, k_1 and k_2 are to be specified, where α is the expected proportion of active factors, k_1 is the expected size of the main effect of an active factor relative to an inert contrast, and k_2 the expected size of a two-factor interaction among active factors relative to an inert contrast.

To estimate plausible values for α, k_1 and k_2, the published examples given in Box and Meyer (1986) Table 1 are reexamined. For each example, α is estimated by the proportion of factors declared active by the authors, k_1^2 is estimated by the mean squared main effect among active factors over the mean squared inert contrast, and k_2^2 is estimated by the mean squared two-factor interaction among active factors over the mean squared inert contrast. In this context not all active contrasts will be large, although all inert contrasts should be small. The estimated values of α, k_1 and k_2 are presented in Table 1.

For those examples which are full factorials and the one which is a half-fraction, at least half of the variables were declared active. For the more highly fractionated designs, of course, a much smaller proportion of the variables were found to be active. Thus the value of α to be specified in any particular situation depends on the degree of fractionation of the design, or more correctly, the degree of fractionation will depend on the experimenter's expectation of the number of important factors, which would also be reflected in the value of α. For full factorials or half-fractions, a reasonable range for α would be from 0.4 to 0.8, while for more fractionated screening designs, the range would be reduced to 0.2 to 0.4.

In all but one example the value of k_1 for main effects is larger than k_2 for two-factor interactions, and the ratio of the average k_1 to the average k_2 is 3.33.

Example	n	fraction	α	k_1	k_2
BHH p. 398	16	1/16	.38	9.3	6.5
BHH p. 327	16	1	.75	15.2	2.7
BHH p. 378	32	1	.60	11.8	8.9
Davies p. 274	16	1	.50	1.9	2.5
Davies p. 462	16	1/2	.80	7.6	2.2
Daniel p. 71	16	1	.75	13.0	1.0
BF p. 557	16	1	.75	26.8	6.3
JL p. 183	32	1	.60	3.0	1.1
JL p. 196	16	1	.75	11.9	1.5
TW p. 69	16	1/32	.22	9.5	$\ll 1.0$
Average		low	.69	11.0	3.3
		high	.30		

Table 1. Estimated values of α, k_1 for main effects and k_2 for interactions for the modified model, from published examples of two-level experiments taken from Box, Hunter and Hunter (1978), Davies ed. (1954), Daniel (1976), Bennett and Franklin (1954), Johnson and Leone (1964), and Taguchi and Wu (1980). In Daniel's example the analysis is conducted after making a log transformation in the response.

4. Examples

The analysis is illustrated in this section with an example, the 2^{8-4} injection molding example from Box, Hunter and Hunter (1978). The factors, their allocation to the 16×16 design array, and the vector of observations are given in Table 2, along with the vector of estimated effects and their respective alias strings. Recall that in Box and Meyer (1986) it was shown that column contrasts 4, 12 and 13 were very likely active, each receiving posterior probability close to one. There was also weak evidence to suggest contrast 8 might also be active. Assuming interactions between three or more factors to be inert, contrasts 8, 12 and 13 are associated with the main effects of factors 1 (screw speed), 5 (holding pressure) and 6 (booster pressure). The large contrast of column 4 is associated with the sum of four two-factor interactions denoted by the alias string 15 + 26 + 37 + 48. Box, et al., suggested that it was most likely either the 15 or 26 interaction which would explain the large contrast, because these involved variables with large main effects. They described a four-run follow-up experiment in which separate estimates of the four interactions were obtained, and deduced that the 15 interaction was indeed the major component of the aliased contrast.

The posterior probabilities that each factor is active were computed with $\alpha = 0.3$, $k_1 = 11$ and $k_2 = 3.3$ and are presented in Table 3, again assuming that interactions between three or more factors are inert. Factors 1 (screw speed), 5 (holding pressure) and 6 (booster pressure) have posterior probabilities close to one and could plausibly be considered active. Factor 2 (temperature) has posterior probability of 0.4, with all other factors receiving very small values. Examination of the alias strings of Table 2 suggests why factor 2 receives non-negligible posterior probability. Although it does not have a large main effect, the two largest interactions could be

Factors

1	(S)	Screw speed
2	(T)	Temperature
3	(M)	Moisture
4	(V)	Thickness
5	(H)	Holding pressure
6	(B)	Booster pressure
7	(C)	Cycle time
8	(G)	Gate size

Column allocation

									S	T	M	V	H	B	C	G	Y
	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	
1	+	-	-	+	-	+	+	-	-	+	+	-	+	-	-	+	14.0
2	+	+	-	-	-	-	+	+	-	-	+	+	+	+	-	-	16.8
3	+	-	+	-	-	+	-	+	-	+	-	+	+	-	+	-	15.0
4	+	+	+	+	-	-	-	-	-	-	-	-	+	+	+	+	15.4
5	+	-	-	+	+	-	-	+	-	+	+	-	-	+	+	-	27.6
6	+	+	-	-	+	+	-	-	-	-	+	+	-	-	+	+	24.0
7	+	-	+	-	+	-	+	-	-	+	-	+	-	+	-	+	27.4
8	+	+	+	+	+	+	+	+	-	-	-	-	-	-	-	-	22.6
9	+	-	-	+	-	+	+	-	+	-	-	+	-	+	+	-	22.3
10	+	+	-	-	-	-	+	+	+	+	-	-	-	-	+	+	17.1
11	+	-	+	-	-	+	-	+	+	-	+	-	-	+	-	+	21.5
12	+	+	+	+	-	-	-	-	+	+	+	+	-	-	-	-	17.5
13	+	-	-	+	+	-	-	+	+	-	-	+	+	-	-	+	15.9
14	+	+	-	-	+	+	-	-	+	+	-	-	+	+	-	-	21.9
15	+	-	+	-	+	-	+	-	+	-	+	-	+	-	+	-	16.7
16	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	20.3

column	contrast	alias string
1	-0.3	12 + 34 + 56 + 78
2	-0.2	13 + 24 + 57 + 68
3	-0.3	14 + 23 + 58 + 67
4	2.3	15 + 26 + 37 + 48
5	0.45	16 + 25 + 38 + 47
6	-0.1	17 + 28 + 35 + 46
7	-0.15	18 + 27 + 36 + 45
8	-0.6	1
9	0.35	2
10	0.05	3
11	0.15	4
12	-2.75	5
13	1.9	6
14	0.05	7
15	-0.3	8

Table 2. Factors, column allocation to the standard 16-run two-level factorial design, observations, estimated effects and alias strings for Example 1.

	Factor	Posterior probability
1	(S) Screw speed	.875
2	(T) Temperature	.400
3	(M) Moisture	.002
4	(V) Thickness	.004
5	(H) Holding pressure	1.000
6	(B) Booster pressure	.998
7	(C) Cycle time	.003
8	(G) Gate size	.009

Table 3. Posterior probabilities p^* that factors are active, Example 1 with $\alpha = 0.3$, $k_1 = 11$, and $k_2 = 3.3$.

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explained by the effect of variable 2 (as well as variable 1) interacting with the active factors 5 and 6. Variable 1 received higher posterior probability because of its larger main effect.

Alternatively, if variables 1, 5 and 6 were truly the active factors, there is one other variable which would be difficult to separate from those three, and that is variable 2. The design collapses into a full factorial in any combination of four factors which includes variables 1, 5 and 6 <u>except</u> the combination 1, 2, 5 and 6, for which the design collapses into a replicated half fraction. Thus the three two-factor interactions among the variables 1, 5 and 6 are confounded with the three two-factor interactions between 1, 5 and 6 and variable 2. The structure of the design dictates that, given that 1, 5 and 6 are the active factors, it will be more difficult to accumulate evidence against variable 2 than the remaining four factors. This phenomenon is reflected in the results of the analysis.

In Figure 1 the posterior probabilities are plotted as a bar plot, with boxes indicating the range for each probability over different combinations of $\alpha = 0.2$, 0.3 and 0.4, $k_1 = 5$, 11, and 15, and $k_2 = 2$, 3.3 and 6, only taking those combinations with $k_1 > k_2$. The posterior probability for factor 2 is the only one that changes enough to affect conclusions about the experiment. Conclusions about this factor depend upon assumptions about the frequency of active factors and the relative size of main effects, interactions and inert contrasts, and these assumptions are reflected in the values of α, k_1 and k_2. In particular, if knowledge of these parameters is vague, variable 2 cannot be safely eliminated.

Suppose now that the assumption that three-factor interactions are inert is dropped. Although this is a very reasonable assumption in practice, it will be interesting to observe what occurs in its absence. The posterior probabilities of the factors were recomputed based on the new set of assumptions and are presented in Table 4. The evidence for variables 5 and 6 is still strong, but the posterior probabilities for variables 1 and 2 are now almost equal. The reason can be found in the revised alias strings for each contrast in Table 4. The contrast associated with the main effect of variable 1 is confounded with the 256 interaction. Now that this contrast, which is too large to attribute entirely to noise, can be associated with an effect of variables 2, 5 and 6, the evidence for variable 2 is stronger, and the evidence for variable 1 is somewhat weaker. This alternative analysis was presented to demonstrate that an experimenter who might have eliminated variable 2 based on the previous analysis would have depended heavily on the assumption that three-factor interactions were inert.

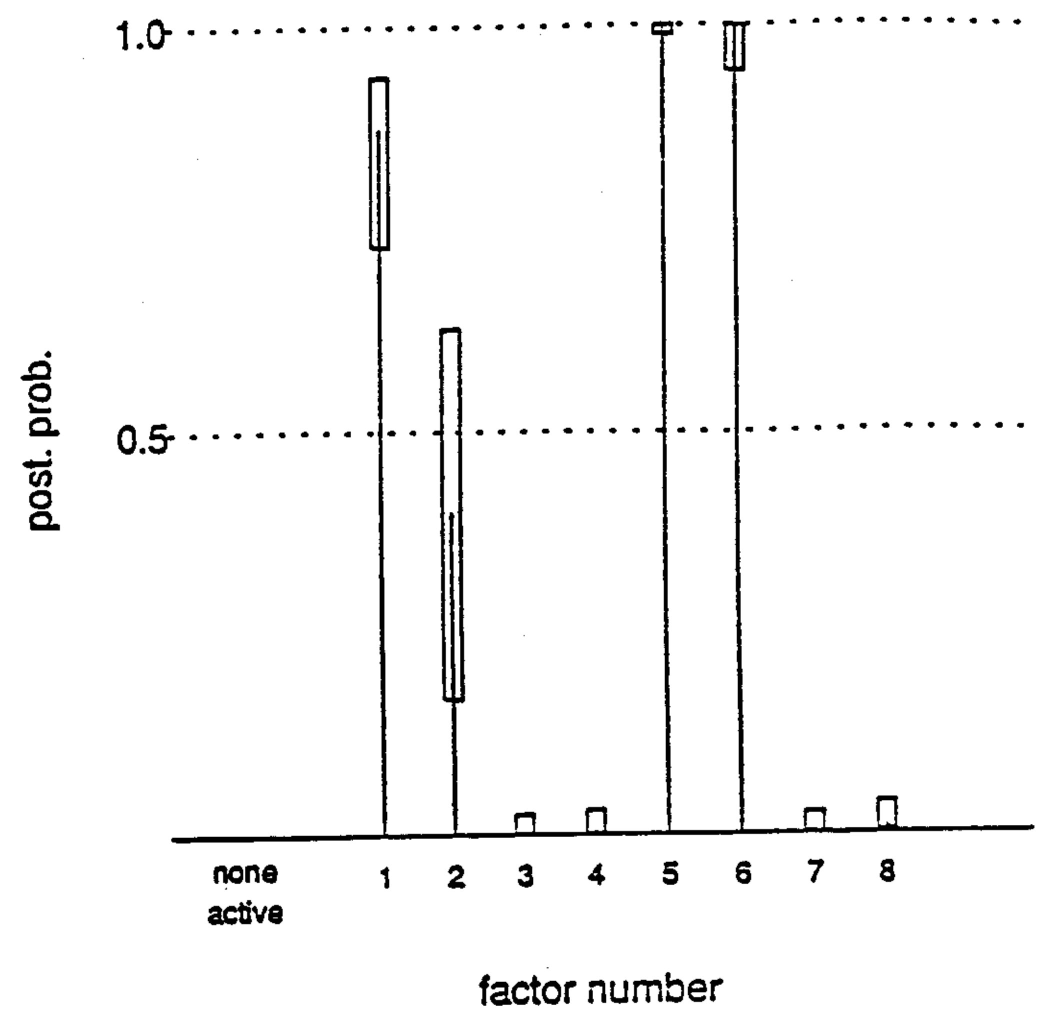

Figure 1. Posterior probabilities $\{p_i^*\}$ that factors are active, Example 2.1. Solid lines indicate values for $\alpha = 0.3$, $k_1 = 11$, $k_2 = 3.3$, boxes indicate range of values for different combinations of $\alpha = 0.2, 0.3, 0.4$, $k_1 = 5, 11, 15$, and $k_2 = 2, 3.3, 6$.

There are two separate issues to consider when making assumptions: the reasonability of the assumptions, and the dependence of the conclusions on the assumptions. It was shown in this example that conclusions are sensitive to the assumption that three-factor interactions are inert. While the reasonability of this assumption is not questioned, it is important to know when conclusions depend on assumptions even when they are well-based.

	Factors	Posterior probability
1	(S) Screw speed	.608
2	(T) Temperature	.537
3	(M) Moisture	.000
4	(V) Thickness	.000
5	(H) Holding pressure	.991
6	(B) Booster pressure	.942
7	(C) Cycle time	.000
8	(G) Gate size	.000

column	contrast	alias string
1	-0.3	12 + 34 + 56 + 78
2	-0.2	13 + 24 + 57 + 68
3	-0.3	14 + 23 + 58 + 67
4	2.3	15 + 26 + 37 + 48
5	0.45	16 + 25 + 38 + 47
6	-0.1	17 + 28 + 35 + 46
7	-0.15	18 + 27 + 36 + 45
8	-0.6	1 + 256
9	0.35	2 + 156
10	0.05	3
11	0.15	4
12	-2.75	5 + 126
13	1.9	6 + 125
14	0.05	7
15	-0.3	8

Table 4. Posterior probabilities p^* that factors are active, Example 1, with $\alpha = 0.3$, $k_1 = 11$, $k_2 = 3.3$, allowing for the possibility of three-factor interactions. Revised aliased strings showing three-factor interactions among 1, 2, 5 and 6 are given.

To demonstrate further the point made about confounding when there are $R - 1$ active factors for a design of resolution R, consider the following exercise. Suppose the three factors 1, 5 and 6 were the only active factors. Their activity could be manifested in several different combinations of main effects and interactions. Assuming the 156 interaction is inert, that leaves three main effects and three two-factor interactions among the active factors. For purposes of illustration, artificial data will be created to explore the relationships among the factors 1, 2, 5 and 6 under these circumstances.

Suppose main effects take on the values 2 or 0, and two-factor interactions are either 1 or 0. Since each effect can take on either of two values, there are $2^6 = 64$ possible combinations of main effects and interactions. For each combination, a vector of observations $\underset{\sim}{y}$ is generated, with no error component, and the posterior probabilities $\{p_i^*\}$ are computed, with $\alpha = 0.3$, $k_1 = 11$ and $k_2 = 3.3$.

Of the 64 possible combinations of the six effects, 23 correspond to situations when not all three factors are active, for example when all six effects are zero, or when the main effect of factor 5 is the only nonzero effect. These are eliminated from further consideration. The remaining $64 - 23 = 41$ can be represented by 12 distinct combinations. For example, there are three ways to have three nonzero main effects and one nonzero interaction, but each of these gives the same pattern of values for the posterior probabilities. The 12 distinct combinations and the probabilities $\{p_i^*\}$ for factors 1, 2, 5 and 6 are presented in Table 5. (The remaining factors received posterior probability of zero, to two decimal places, for all 12 combinations.)

As seen in the table, there are many situations in which factor 2 receives significant posterior probability, despite the fact it is actually inert and there is no error component in the data. The combinations for which it was easiest to detect the truly active factors were those in which all main effects were large. As main effects were dropped it became more difficult to separate factor 2 from the other three factors. This is because the assumption that main effects are larger and occur more frequently than interactions has been incorporated into the model, and situations for which this does not hold can lead to these unexpected patterns of probabilities. However, on the premise that the assumption about main effects is basically sound, these troublesome situations should not be frequent. Note also there was only one combination where active factors did not receive large probabilities, and this was the combination where there was a nonzero interaction between factors 5 and 6, but their respective main effects were zero.

Effects						Posterior Probabilities			
1	5	6	15	16	56	1	2	5	6
2	2	2	0	0	0	1.00	.01	1.00	1.00
2	2	2	1	0	0	1.00	.09	1.00	1.00
2	2	2	1	1	0	1.00	.21	1.00	1.00
2	2	2	1	1	1	1.00	.30	1.00	1.00
2	2	0	0	1	0	1.00	.54	1.00	.54
2	2	0	1	1	0	1.00	.59	1.00	.59
2	2	0	0	1	1	1.00	.59	1.00	.59
2	2	0	1	1	1	1.00	.62	1.00	.62
2	0	0	1	1	0	1.00	.74	.74	.74
2	0	0	1	0	1	1.00	.74	.74	.74
2	0	0	1	1	1	1.00	.76	.76	.76
2	0	0	0	0	1	1.00	.99	.01	.01

Table 5. Posterior probabilities of factors being active over the 12 distinct combinations of active effects for the active factors 1, 5 and 6, $\alpha = 0.3$, $k_1 = 11$, $k_2 = 3.3$.

Two conclusions are apparent from this exercise. First, when there are $R - 1$ active factors in a design of resolution R, it is sometimes not possible to identify the correct factors exactly, even though the design projects into a full factorial in the R - 1 factors. Fortunately, it will usually be possible to restrict attention to some subset of variables, and it would be rare that active factors would be excluded from this subset due to inherent properties of the design and analysis (active factors may be concealed by noise). In the example above it was possible to restrict attention to four of the original eight variables. A follow-up experiment such as the one described in Box, Hunter and Hunter (1978), p. 413, can be implemented to eliminate any remaining inert factors. Second, the Bayesian analysis provides a good method for identifying the likely subset of variables by combining prior assumptions, properties of the experimental design and information in the data. Factors such as factor 2 in the above example which cannot be safely eliminated because of the structure of the design, as well as those factors which are more obviously active, are identified by their non-negligible posterior probability.

5. Conclusions

The small number of runs per factor in a fractional factorial usually makes it impossible to specify only one possible explanation for the observed data, but the number of possible explanations can be reduced at each round of experimentation with fewer total runs than one supposedly comprehensive experiment. The information needed to eliminate possible explanations can come from two sources, prior knowledge of the system and experimental data. Any good statistical analysis used to identify likely or unlikely explanations will utilize information from both sources. A good statistical analysis will also contain some measure of sensitivity to uncertainty in this information. The computation of posterior probabilities for the purpose of identifying active factors has been shown to depend on prior assumptions, design properties and of course experimental data. In particular, factors which cannot be eliminated due to the confounding structure of the design are identified by a non-negligible posterior probability. By the implementation and subsequent withdrawal of various assumptions the sensitivity of this method to assumptions can also be assessed.

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