LOCATION AND DISPERSION EFFECT INFERENCE IN UNREPLICATED FRACTIONAL FACTORIAL DESIGNS

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1 Introduction

Traditionally, the primary use of fractional factorial designs has been in detecting the factors that produce location effects (changes in the mean response). An assumption of constant variance (no dispersion effects) is usually made. If a factor produces a dispersion effect in the response, this effect can be exploited to reduce the variation in a manufactured product. Thus, identifying and studying dispersion effects can result in a product or process that is robust to environmental variations (noise).

For unreplicated fractional factorials however, there is no estimate of variation available at each design setting, making the study of dispersion effects more challenging. If the design is a fractional (not full) factorial, the confounding greatly increases the complexity. What has not been adequately discussed in the literature is how to study location effects in the presence of one or more dispersion effects in highly fractionated unreplicated designs.

In this paper, we will develop the exact relationship between location and dispersion effects. Specifically, we will show that pairs of location effects are correlated in the presence of a dispersion effect. An estimate of the dispersion effect magnitude will be developed and used to estimate the correlation between location effect estimates. In addition, we will recommend a step-by-step procedure for estimating both location and dispersion effects in unreplicated 2^{k-p} experiments.

2 Location Effect Confounding

Suppose an $n = 2^{k-p}$ fractional factorial design is run. Here, the design matrix, $X = (\mathbf{x_0}, \mathbf{x_1}, \ldots, \mathbf{x_{n-1}})$ represents k factors and possibly interactions between these factors depending

on the degree of fractionization, $\mathbf{x_0} = (1, \ldots, 1)'$, and $(\mathbf{x_j} = x_{1j}, x_{2j}, \ldots, x_{nj})'$ with $x_{ij} = \pm 1$, $j = 1, \ldots, n-1$. Making the usual assumptions, we have $Y_i = \sum_{j=0}^{n-1} x_{ij}\beta_j + \epsilon_i$, $\epsilon_i \sim N(0, \sigma^2)$ with Y_i's being independent observations. When there are no dispersion effects, $Var(Y_i) = Var(\epsilon_i) = \sigma^2$. However, suppose column $\mathbf{x_d}$ produces a dispersion effect as follows: $Var(Y_i | i \in M) = \sigma_{d-}^2$, $Var(Y_i | i \in P) = \sigma_{d+}^2$, and $\Delta = \sigma_{d+}^2/\sigma_{d-}^2$ where M is the set of rows where $x_{id} = -1$ and P is the set of rows where $x_{id} = +1$, i.e. $M =$ minus, $P =$ plus. Let columns $\mathbf{x_j}$ and $\mathbf{x_{j'}}$ be any pair of columns whose interaction is in column $\mathbf{x_d}$. (There are $(n-2)/2$ of these pairs, referred to hereafter as "alias pairs.") Then $x_{ij}x_{ij'} = x_{id}$. Let $\hat{\beta}_j$ and $\hat{\beta}_{j'}$ be the ordinary least squares (OLS) estimators of β_j and $\beta_{j'}$, the regression coefficients associated with $\mathbf{x_j}$ and $\mathbf{x_{j'}}$ respectively.

Theorem 1 *Let $\hat{\beta}_j$ and $\hat{\beta}_{j'}$ be the OLS estimates for columns $\mathbf{x_j}$ and $\mathbf{x_{j'}}$ respectively in a 2^{k-p} experiment. If the interaction of $\mathbf{x_j}$ and $\mathbf{x_{j'}}$ is in column $\mathbf{x_d}$, $Var(\epsilon_i | x_{id} = -1) = \sigma_{d-}^2$ and $Var(\epsilon_i | x_{id} = 1) = \sigma_{d+}^2$, then the correlation of $\hat{\beta}_j$ and $\hat{\beta}_{j'}$ is*

$$\rho_{j,j'|d} = \frac{\sigma_{d+}^2 - \sigma_{d-}^2}{\sigma_{d+}^2 + \sigma_{d-}^2}. \tag{1}$$

Proof: Available upon request.

Simulations were performed and they confirm what may be intuitive in light of the this correlation. The individual power of a location effect is not affected by the dispersion-induced correlation but the joint power of two tests is. Therefore, if there is any question that an effect is active when its alias is, we should tentatively include both in the location model. In the following sections we discuss testing for dispersion effects and how to incorporate the dispersion-induced correlation in location effect estimation.

3 Dispersion Estimates and Tests

We now develop a dispersion effect test statistic. Assume a location model is fit with m location effects (plus the overall mean) and residuals are calculated where e_i = residual of observation i. For column x_d, define the following: $s_{d+}^2 = \frac{2}{n-2}\sum_{i\in P}(e_i - \bar{e}_p)^2$ and $s_{d-}^2 = \frac{2}{n-2}\sum_{i\in M}(e_i - \bar{e}_m)^2$ where $\bar{e}_p = (2/n)\sum_{i\in P}e_i$ and $\bar{e}_m = (2/n)\sum_{i\in M}e_i$. Suppose the effect matrix of an adapted location model consists exactly of $x_0 = 1$, x_d, and pairs of columns $(x_j, x_{j'})$ such that the interaction of x_j and $x_{j'}$ is in column x_d. This is the condition for using Bergman and Hynén's (1997) D^{BH} test.

Theorem 2 *Let m be the number of active location effects in the model fit from a 2^{k-p} experiment. Let g = the number of alias pairs $(x_j, x_{j'})$ not in the model such that $x_{ij}x_{ij'} = x_{id}$ for $i = 1, \ldots, n$. Then s_{d+}^2 and s_{d-}^2 are independent if and only if $g = (n - 1 - m)/2$ and x_d is in the effect matrix for the fitted model.*

Corollary 1 *Under the conditions of Theorem 2 and allowing for a possible dispersion effect in column d with $Var(Y_i|i \in M) = \sigma_{d-}^2$ and $Var(Y_i|i \in P) = \sigma_{d+}^2$,*

$$\frac{(n-2)s_{d+}^2}{2\sigma_{d+}^2} \text{ and } \frac{(n-2)s_{d-}^2}{2\sigma_{d-}^2} \sim \chi_g^2 \quad independently. \quad (2)$$

Under $H_0 : \sigma_{d+}^2 = \sigma_{d-}^2$,

$$F = s_{d+}^2/s_{d-}^2 \sim F_{(g,g)} \quad (3)$$

Proofs: Available upon request.

Thus we see that to properly perform dispersion effect testing, a different location model may need to be fit for each column to be tested. In addition, recall that in section 2 we showed that a dispersion effect creates a correlation $(\rho_{j,j'|d})$ among pairs of location effect estimates. We can now find independent estimators of σ_{d+}^2 and σ_{d-}^2 and suggest an estimator of $\rho_{j,j'|d}$. Let

$$r_d = (s_{d+}^2 - s_{d-}^2)/(s_{d+}^2 + s_{d-}^2). \quad (4)$$

It can be shown that, under the conditions of Theorem 2, r_d is the maximum likelihood estimator estimator of $\rho_{j,j'|d}$.

We next explore the impact of multiple dispersion effects. Define an interaction triple $(x_j, x_{j'}, x_{j''})$ such that $x_{ij}x_{ij'} = x_{ij''}$. Define the actual magnitude of dispersion effects in these columns as Δ_j, $\Delta_{j'}$ and $\Delta_{j''}$. Suppose there are exactly two of these columns

Figure 1: Welding Experiment Location Effect Plots

a) Normal Plot of Welding Coefficients   b) Half-Normal Plot of Welding Coefficients
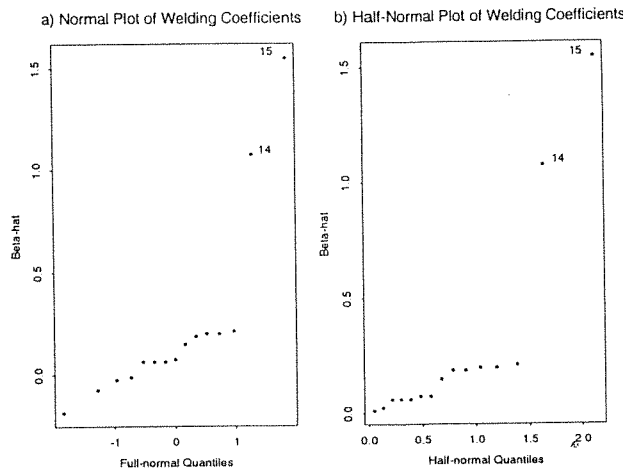
having dispersion effects ($\Delta \neq 1$). Then a dispersion effect is induced in their interaction column (the third member of the interaction triple) which, in turn, induces a correlation among this column's location alias pairs. For example, letting $\Delta_{j''}^I$ be the dispersion effect induced by the other two dispersion effects, it can be shown that

$$\Delta_{j''}^I = (1 + \Delta_j\Delta_{j'})/(\Delta_j + \Delta_{j'}). \quad (5)$$

4 Example 1

As an example, we will use data analyzed by Box and Meyer (1986) among others. The data from this welding experiment performed by the National Railway of Japan were originally analyzed in Taguchi and Wu (1980). Table 1 displays the design matrix and data for this 2^{9-5} fractional factorial design. The factors are labeled in the "W" row of this table and the response (tensile strength) is in the y_W column. Normal and half-normal plots (see Daniel (1959)) of the OLS estimates are shown in Figure 1. Here the column 14 and the column 15 (x_{14} and x_{15}) location effects appear active. Box and Meyer fit this location model and calculated residuals. To study dispersion effects, they calculated the natural logarithm of the ratio of sample variances for their model and stated that this statistic has an approximate normal distribution. Based on this statistic, the largest apparent dispersion effect is in column 15 with $s_{15+}^2 = 0.524$ and $s_{15-}^2 = 0.028$. From this they concluded that column 15 has a dispersion effect.

This dispersion effect produces the following alias pairs: 1:14, 2:13, 3:12, 4:11, 5:10, 6:9, 7:8 . Using (4)

Table 1: Experimental Designs ($2^{k-p} = 16$) and Responses

W		D	H	G	A		-F	-E						J	B	-C		
AM		A	B	C	D											E		
	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	y_W	y_{AM}
1	1	-1	-1	-1	-1	1	1	1	1	1	1	-1	-1	-1	-1	1	43.7	13
2	1	1	-1	-1	-1	-1	-1	-1	1	1	1	1	1	1	-1	-1	40.2	54
3	1	-1	1	-1	-1	-1	1	1	-1	-1	1	1	1	-1	1	-1	42.4	44
4	1	1	1	-1	-1	1	-1	-1	-1	-1	1	-1	-1	1	1	1	44.7	49
5	1	-1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1	1	-1	42.4	13
6	1	1	-1	1	-1	-1	1	-1	-1	1	-1	-1	1	-1	1	1	45.9	14
7	1	-1	1	1	-1	-1	-1	1	1	-1	-1	-1	1	1	-1	1	42.2	18
8	1	1	1	1	-1	1	1	-1	1	-1	-1	1	-1	-1	-1	-1	40.6	85
9	1	-1	-1	-1	1	1	1	-1	1	-1	-1	-1	1	1	1	-1	42.4	41
10	1	1	-1	-1	1	-1	-1	1	1	-1	-1	1	-1	-1	1	1	45.5	73
11	1	-1	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1	-1	1	43.6	79
12	1	1	1	-1	1	1	-1	1	-1	1	-1	-1	1	-1	-1	-1	40.6	17
13	1	-1	-1	1	1	1	-1	-1	-1	-1	1	1	1	-1	-1	1	44.0	82
14	1	1	-1	1	1	-1	1	1	-1	-1	1	-1	-1	1	-1	-1	40.2	58
15	1	-1	1	1	1	-1	-1	-1	1	1	1	-1	-1	-1	1	-1	42.5	10
16	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	46.5	29

we have $r_{15} = (0.524 - 0.028)/(.524 + .028) = .897$. Thus location effect estimates within each of these pairs appear to be highly correlated. However, the conditions of Theorem 2 are not met. For the fitted location model, $(n - 1 - m)/2 = 6.5$ and $g = 6$ because the alias of column 14, i.e. column 1, is not in the model. Thus, the estimate of the dispersion effect and its induced correlation among location effects are under estimated. To perform an exact test for a dispersion effect in column 15, we must first fit a different model. Including the appropriate alias into the model we have $\hat{y}_i = \hat{\beta}_0 + x_{i1}\hat{\beta}_1 + x_{i14}\hat{\beta}_{14} + x_{i15}\hat{\beta}_{15}$. To test for dispersion effects in the other columns, the location model was adapted in the appropriate manner. From this analysis, in addition to the dispersion effect in column 15, we find active dispersion effects in column 2 ($F_2 = 15.93$, p=.0086) and 13 ($F_{13} = 20.96$, p=.0046).

Notice that these three columns form an interaction triple. It is not possible to determine if only two or all three are active. If we assume, however, that the two largest are active (columns 13 and 15), then we can estimate the induced dispersion effect in column 2. With $\hat{\Delta}_{13} = F_{13} = 20.96$ and $\hat{\Delta}_{15} = F_{15} = 21.72$ we have $\hat{\Delta}_2^{(I)} = (1 + (20.96)(21.72))/(20.96 + 21.72) = 10.69$. So if columns 13 and 15 truly have dispersion effects of the observed magnitude, then the expected effect in column 2 is more than ten times the actual dispersion effect magnitude. The observed column 2 effect of $F_2 = 15.93$ indicates that this dispersion effect is probably spurious if the other two are active. Of course the same form of relationship holds for the other two columns. So it seems that two of these columns have dispersion effects but we can not determine which two! Additional investigation in this area is needed to fully study location effect estimation with consideration of multiple dispersion effects.

5 Estimation and Significance of Location Effects

We now develop a method of estimating location effects incorporating the correlation among alias pairs. We use the original location effect model as a starting point. All effect estimates that are not in the model and are aliased with another effect that is not in the model are initially assumed inactive. However, a single alias not in the model is correlated with an assumed active effect. Their correlation may have a large impact on the OLS estimates. Thus we will include aliases of "active" effects in the model resulting in Theorem 2 conditions. As all effects in this model are correlated in pairs, we will estimate them in pairs.

Recall that

$$\left(\hat{\beta}_j, \hat{\beta}_{j'}\right) \sim N_2 \left(\begin{pmatrix} \beta_j \\ \beta_{j'} \end{pmatrix}, \frac{1}{2n} \begin{pmatrix} \sigma_{d+}^2 + \sigma_{d-}^2 & \sigma_{d+}^2 - \sigma_{d-}^2 \\ \sigma_{d+}^2 - \sigma_{d-}^2 & \sigma_{d+}^2 + \sigma_{d-}^2 \end{pmatrix} \right).$$

With this bivariate normal distribution, it is straightforward to show

$$\frac{n(\sigma_{d+}^2 + \sigma_{d-}^2)}{2\sigma_{d+}^2\sigma_{d-}^2} \times \left[\left(\hat{\beta}_j - \beta_j \right)^2 \right.$$

$$\left. -2\frac{\sigma_{d+}^2 - \sigma_{d-}^2}{\sigma_{d+}^2 + \sigma_{d-}^2} \left(\hat{\beta}_j - \beta_j \right) \left(\hat{\beta}_{j'} - \beta_{j'} \right) + \left(\hat{\beta}_{j'} - \beta_{j'} \right)^2 \right] \sim \chi_2^2.$$

Of course, σ_{d+}^2 and σ_{d-}^2 are unknown. However,

$$\frac{n-2}{2} \left(\frac{s_{d+}^2}{\sigma_{d+}^2} + \frac{s_{d-}^2}{\sigma_{d-}^2} \right) = \frac{n-2}{2} \left(\frac{s_{d+}^2\sigma_{d-}^2 + s_{d-}^2\sigma_{d+}^2}{\sigma_{d+}^2\sigma_{d-}^2} \right) \sim \chi_{2g}^2$$

from (2). As s_{d+}^2 and s_{d-}^2 are functions of the location effect estimates that are not in the model, they are independent of $\hat{\beta}_j$ and $\hat{\beta}_{j'}$ which are in the model. Therefore,

$$\frac{ng}{n-2} \left(\frac{\sigma_{d+}^2 + \sigma_{d-}^2}{s_{d+}^2\sigma_{d-}^2 + s_{d-}^2\sigma_{d+}^2} \right) \times \left[\left(\hat{\beta}_j - \beta_j \right)^2 \right.$$

$$\left. -2\frac{\sigma_{d+}^2 - \sigma_{d-}^2}{\sigma_{d+}^2 + \sigma_{d-}^2} \left(\hat{\beta}_j - \beta_j \right) \left(\hat{\beta}_{j'} - \beta_{j'} \right) + \left(\hat{\beta}_{j'} - \beta_{j'} \right)^2 \right] \sim F_{2,2g}.$$
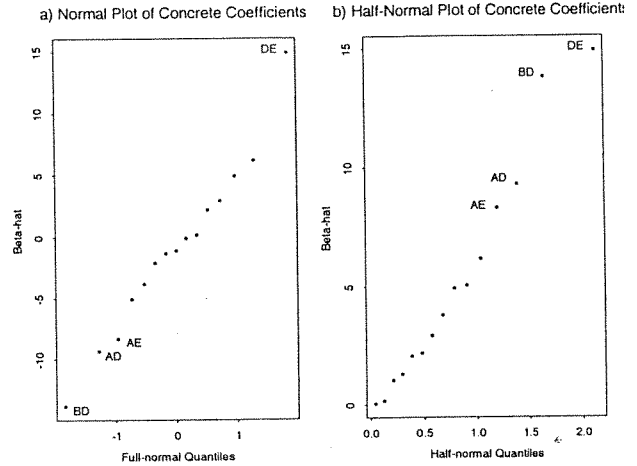
Unfortunately, σ_{d+}^2 and σ_{d-}^2 are not removed. If they were known, $100(1-\alpha)\%$ confidence regions for $(\hat{\beta}_j, \hat{\beta}_{j'})$ could be calculated by equating the left side above to $F_{2,2g}(1-\alpha)$. If, for a given α, this elliptical region includes values of $\beta_j = 0$, then the location effect would not be considered active. As it does not appear an exact confidence region is possible, we will approximate this region using $\hat{\sigma}_{d+}^2 = (n-2)s_{d+}^2/2g$ and $\hat{\sigma}_{d-}^2 = (n-2)s_{d-}^2/2g$. As these are unbiased estimators, we have an unbiased estimate of the joint confidence region,

$$(s_{d+}^2 + s_{d-}^2)(\hat{\beta}_j - \beta_j)^2 - 2(s_{d+}^2 - s_{d-}^2)(\hat{\beta}_{j'} - \beta_{j'})(\hat{\beta}_j - \beta_j)$$

$$+(s_{d+}^2 + s_{d-}^2)(\hat{\beta}_{j'} - \beta_{j'})^2 - \frac{2(n-2)}{ng}s_{d+}^2 s_{d-}^2 F_{2,2g} = 0. \quad (6)$$

6 Example 2

As another example, we look at data originally analyzed by Anderson and McLean (1974). The experiment was a 2^{5-1} design to study the impact of five factors on an index of "goodness" of asphalt concrete. The response is shown in the y_{AM} column of Table 1 and the factors are labeled in the "AM" row. Anderson and McLean use an *a priori* estimate of 200 for the error mean square and found four effects to be found active: AD, AE, BD, and DE. Note that none of the active effects are main effects.

Without a previous estimate of the error variance, some terms would need to be considered inactive in order to form an error term. To separate the active and inactive location effects, we use the normal and

Figure 2: Concrete Location Effect Plots

a) Normal Plot of Concrete Coefficients   b) Half-Normal Plot of Concrete Coefficient

half-normal plots in Figure 2. This method is subjective. One logical interpretation of four active location effects (AD, AE, BD and DE) seems to agree with McLean and Anderson's findings. Also, fitting this location model results in a mean square error of 179.5, reasonably close to the pre-experiment estimate of 200. Table 2 shows the sample variances, F statistics based on (3), and associated p-values for this four location effect model. We see that AB and E have mildly significant dispersion effects with p-values of .0567 and .0424 respectively.

Table 2: Concrete Dispersion Statistics

Column	s_{d-}^2	s_{d+}^2	F	p-value
A	52.21	7.34	0.14	0.1413
B	52.71	60.91	1.16	0:9082
C	110.43	134.36	1.22	0.8757
D	40.79	74.77	1.83	0.6310
AB	220.14	24.64	0.11	0.0567
AC	129.29	60.91	0.47	0.5523
AD	69.29	208.80	3.01	0.2513
BC	60.79	57.34	0.94	0.9629
BD	179.57	65.21	0.36	0.3502
CD	154.07	37.34	0.24	0.2748
DE	128.29	153.66	1.20	0.8478
CE	111.21	34.20	0.31	0.3586
BE	63.00	181.79	2.89	0.3292
AE	145.87	126.44	0.87	0.8792
E	5.36	93.05	17.37	0.0424

Recall that if both of these dispersion effects are active, then a dispersion effect is induced in their interaction column. The interaction of AB and E appears in CD. Using (5) we have $\hat{\Delta}_{CD}^I = (1 +$

$(.11)(17.37))/(.11 + 17.37) = 0.17$. Also, $\Delta_{CD}^{E} = \Delta_{CD}\Delta_{CD}^{I}$ where Δ_{CD}^{E} is the expected observed dispersion effect magnitude. Substituting the observed value of 0.24 from Table 2 for Δ_{CD}^{E} and solving for Δ_{CD} we have a conditional estimate of the actual dispersion effect, $\hat{\Delta}_{CD} = 0.24/0.17 = 1.4$. This magnitude of dispersion effect is clearly not significant. Thus, if both AB and E have active dispersion effects, they do not appear to mask any dispersion effect in CD.

As a result of meeting Theorem 2 conditions, the p-value for AB is based on 4 and 4 degrees of freedom. Its F statistic suggests that the variance is $1/.11=9.09$ times higher at the low level than at the high level. Similarly, the p-value for E is based on 3 and 3 degrees of freedom and its F statistic suggests the variance is 17.37 times larger at the high level of E than at the low level. While both AB and E may have active dispersion effects, there is more evidence of a dispersion effect in E than in AB. Also, we are more likely to see a main dispersion effect than an interaction dispersion effect. Accordingly, to illustrate location effect estimation in the presence of a single dispersion effect, we will assume E is the only active dispersion effect.

To study the location effect estimates in pairs, we construct confidence region plots using (6). Figure 3 shows these plots of four of the alias pairs. The smallest ellipse in each plot is the 90% joint confidence region with the mid-sized and largest ellipses being the 95% and 99% regions respectively. If an entire ellipse is on one side of an effects axis, then the p-value is less than the value of α used to create the region. For example, the entire 90% region for AE is below 0 implying the p-value is less than .10. The 95% region just crosses 0 implying the p-value is greater than .05.

One drawback of using these rough p-values is that the joint relationship between aliases is not used. Looking at the A:AE region again, if we assume that A is null (i.e. =0), then the three intervals for AE created by slicing the region at A=0 are all well below 0. Thus, if we believe A is inactive, we also believe AE is active even though its p-value is greater than .05. In a similar manner, if we believe BC=0, then AD is active. Note, however, that its' conditional intervals (slices) are closer to 0 than those of AE indicating less significance.

The D:DE region provides another interesting interpretation. DE is obviously significant but D does not appear to be active as all of the ellipses cross D=0. However, if we assume that the DE loca-

Figure 3: Confidence Region Plots
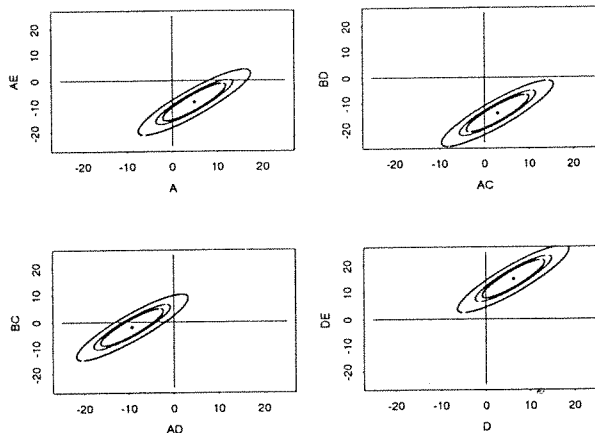
tion effect is the value obtained from the experiment (14.9375) and slice the ellipse at this value, we find that none of the D intervals cross D=0. Thus we may conclude that D is an active location effect if DE=14.9375. This seems reasonable in this experiment as the original four location effects identified were all two-factor interactions, three of which involve D.

So from the above analysis, we may conclude that there are four active two-factor location effect interactions, a location effect due to D, and a dispersion effect due to E. Obviously other interpretations are possible. It seems clear, however, that factor C is not as important as the others. If this truly was a screening experiment, the next round of experimentation should include the other four factors. If some replication is included in this future experiment, it may be possible to more clearly identify the active location and dispersion effects.

7 Summary

In today's modern industry, the extremely short life cycle of products demands efficient and effective use of experimentation to develop the next generation of processes and products. However, with the limited amount of data provided in unreplicated 2^{k-p} fractional factorial experiments (typically 16 or 32 observations), it is quite ambitious to study both location and dispersion effects in a single experiment.

So if we suspect both location and dispersion effects may be present, how do we proceed? We propose an approach exemplified by the example in the previous section.

1. Use a standard procedure, e.g. ANOVA, normal or half-normal plots, or Lenth (1989), to *tentatively* identify active location effects.

2. Fit the reduced model with m location effects and calculate residuals.

3. To test for a dispersion effect in column x_d, determine the alias pattern for $I = x_d$, and calculate g, the number of alias pairs not included in the model.

   (a) If $g = (n-1-m)/2$, then calculate s_{d+}^2 and s_{d-}^2 and perform dispersion effect testing for column x_d using (3).

   (b) If $g \neq (n-1-m)/2$, then add the necessary aliases to the original model in 2) so all terms in the model are in alias pairs. Repeat 2) and 3a).

4. Based on 3a), determine if dispersion effects are present.

   (a) If no dispersion effects are detected, accept that the effects in 1) are the active location effects and stop.

   (b) If one or more dispersion effects are considered active, then create confidence region plots for each pair using (6) and identify location effects now believed to be active.

   (c) Repeat steps 1) - 4) until there is no change in conclusions.

5. Based on 4) include the active dispersion effects in the next round of experimentation.

By deriving the correlation among location effect estimates induced by a dispersion effect, we have shown that these effects should not be studied independently. While ignoring this correlation does not impact the power of an individual location effect test, it does affect the joint power of two such tests.

We have shown that the standard F test may be used on residual variances for dispersion effect testing if all effects in the location model are alias pairs. The test is applicable because the two variances are independent under this condition. If the independence condition is not met, then the ratio of these variances is biased toward 1 making the dispersion effect estimate conservative.

In summary, we recommend that a cyclical approach be used beginning by identifying location effects. As shown by McGrath and Lin (1999a), failure to include a pair of location effects in a model and using residuals to study dispersion can create a spurious dispersion effect. Thus, it is recommended that questionable location effects be tentatively included in the model. If an estimate of variance is available from an external source such as previous data, the error variance from the fitted location model can be compared to this value to see if the location model is reasonable. Alternatively, if all factors are quantitative, center points may be added to the experiment in order to calculate a variance estimate. Residuals from the fitted location model are then used to identify dispersion effects, then the location effects are revisited using joint confidence regions.

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