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Analyzing location and dispersion in unreplicated fractional factorials

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Abstract

We explore the impact of dispersion effects on location effect estimation and derive approximate joint confidence regions for pairs of correlated location effect estimates. A procedure for estimating location effects in the presence of a single dispersion effect is recommended.

Keywords: Confidence regions; Correlation; Experimental design; Variance

1. Introduction

Two-level fractional factorial designs are often used in screening experiments. In these experiments, the goal is to apply the Pareto principle of separating the vital few effects from the trivial many. Many approaches have been developed to study location and dispersion effects when the experiment is replicated. In unreplicated designs, there is no error term to be used for testing if we are interested in estimating effects in all columns. Examples of studying location effects in unreplicated fractional factorial designs include Daniel (1959, 1976), Box and Meyer (1986a), and Lenth (1989). See Hamada and Balakrishnan (1998) for an overview and comparison of different methods.

Others have studied dispersion effects in unreplicated fractional factorials. See Box and Meyer (1986b), Wang (1989), Montgomery (1990), and Bergman and Hynén (1997). Pan (1999), Brenneman and Nair (2001), and McGrath and Lin (2001a) studied the impact of unidentified location effects on dispersion effect identification. What has not been given as much attention in the

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literature is how to study location effects in the presence of dispersion effects in highly fractionated unreplicated designs. Grego et al. (2000) studied the impact of dispersion on normal plotting of location effect estimates. Wolfinger and Tobias (1998) used a mixed model approach which is applicable for unreplicated, but not highly fractionated designs.

In this paper, we recommend a step-by-step procedure for estimating both location and dispersion effects in unreplicated 2^{k-p} experiments. In Section 2 we study the distribution of residual sample variances used to estimate dispersion effects and the correlation induced on location effect estimates by the dispersion effect. In Section 3 we develop new location effect estimation and testing methods when a dispersion effect is present, using an example for illustration. Finally, Section 4 provides a recommended procedure for studying both location and dispersion effects in unreplicated designs.

2. Dispersion effect testing and induced correlation

Suppose an unreplicated $n=2^{k-p}$ fractional factorial design is run. Here, the effect matrix, $\mathbf{X}=(\mathbf{x_0},\mathbf{x_1},\ldots,\mathbf{x_{n-1}})$ represents k factors and possibly interactions between these factors depending on the degree of fractionation, $\mathbf{x_0}=(1,\ldots,1)'$, and $\mathbf{x_j}=(x_{1j},x_{2j},\ldots,x_{nj})'$ with $x_{ij}=\pm 1$, $j=1,\ldots,n-1$. Making the common assumptions (including no dispersion effects), we have

$$Y_i=\sum_{j=0}^{n-1} x_{ij}\beta_j+\varepsilon_i, \quad \varepsilon_i \sim \mathrm{N}(0,\sigma^2)$$

with the ε_i's being independent. (It is assumed that some of the $\beta_j=0$, but these are unknown a priori.) However, suppose column $\mathbf{x_d}$ produces a dispersion effect as follows: $\mathrm{Var}(\varepsilon_i \mid i\in M_d)=\sigma^2_{d-}$ and $\mathrm{Var}(\varepsilon_i \mid i\in P_d)=\sigma^2_{d+}$. Here $M_d=\{i\colon x_{id}=-1\}$ and $P_d=\{i\colon x_{id}=+1\}$. If $\mathbf{x_j}$ and $\mathbf{x_{j'}}$ are any pair of columns whose interaction is in column $\mathbf{x_d}$, then $x_{ij}x_{ij'}=x_{id}$. We will refer to these as dispersion–correlation (dc) pairs. 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.

Box and Meyer (1986b), among others, stated that when attempting to identify dispersion effects, one should first identify location effects and study residuals from the fitted location model. Sample variances of the residuals from the $+1$ and -1 levels of a column, $\mathbf{x_d}$, can be studied to test for a dispersion effect in that column. As these variances are not, in general, independent, their joint distribution is rather complicated. Bergman and Hynén (1997) showed that a traditional F-test can be used to test for dispersion in a given column under a specified condition. Let e_i be the observed residual in row i from a location model. Letting $s^2_{d+}=[2/(n-2)]\sum_{i\in P_d} e_i^2$ and $s^2_{d-}=[2/(n-2)]\sum_{i\in M_d} e_i^2$, Bergman and Hynén (1997) developed a test statistic, $D^{\mathrm{BH}}=s^2_{d+}/s^2_{d-}$ that has an F-distribution if the residuals are calculated from a specific form of location model. To form a Bergman and Hynén (BH) model,

1. record the location model, i.e. the identified location effects and the intercept;
2. adapt the above model, if necessary, to include the location effect of the column to be tested for dispersion and the interaction of this column with each of the others already in the model.

There are $n-2g$ terms in this model and $2g$ terms left out of the model. The e_i are functions of the location effect estimates that are not in the BH model. In fact, they can be calculated based on the dc pairs. Let a dc pair of location effects not in the BH model be denoted j and j' and the pair itself be indexed by $f = 1, \dots, g$. Using this notation, McGrath and Lin (2001a) showed that

$$s_{d+}^2 = \frac{n}{n-2}\sum_{f=1}^{g}\left(\hat{\beta}_j^{(f)} + \hat{\beta}_{j'}^{(f)}\right)^2, \quad s_{d-}^2 = \frac{n}{n-2}\sum_{f=1}^{g}\left(\hat{\beta}_j^{(f)} - \hat{\beta}_{j'}^{(f)}\right)^2. \tag{1}$$

It can be shown from (1) that

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

Under H_0: $\sigma_{d+}^2 = \sigma_{d-}^2$, $D_d^{\mathrm{BH}} = s_{d+}^2/s_{d-}^2 \sim F_{g,g}$.

The presence of one or more dispersion effects complicates location effect estimation. A single dispersion effect induces a correlation among the dc pairs of location estimates. It can be shown that the correlation of $\hat{\beta}_j$ and $\hat{\beta}_{j'}$ is

$$\rho_{j,j'|d} = \frac{\sigma_{d+}^2 - \sigma_{d-}^2}{\sigma_{d+}^2 + \sigma_{d-}^2}. \tag{3}$$

This correlation has been discussed by Grego et al. (2000) and in an unpublished manuscript, Asscher (1991). From (2), it is straightforward to show that

$$r_d = \frac{s_{d+}^2 - s_{d-}^2}{s_{d+}^2 + s_{d-}^2} \tag{4}$$

is the maximum likelihood estimator of $\rho_{j,j'|d}$.

3. Estimation and significance of location effects

So with formal methods for dispersion effect testing, we return to location effect estimation. We want to answer the question "How does the fact that $\hat{\beta}_j$ and $\hat{\beta}_{j'}$ are correlated in the presence of a dispersion effect in column $\mathbf{x_d}$ change their estimation and interpretation?" As all location effect estimates are correlated in pairs in a BH model, we will estimate them in pairs.

With a single dispersion effect in column $\mathbf{x_d}$ and $x_{ij}x_{ij'} = x_{id}, \forall i$,

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

From this bivariate normal distribution, it is straightforward to show that

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

Now σ_{d+}^2 and σ_{d-}^2 are unknown, but from (2) we have $((n-2)/2)(s_{d+}^2/\sigma_{d+}^2 + s_{d-}^2/\sigma_{d-}^2) \sim \chi_{2g}^2$. As s_{d+}^2 and s_{d-}^2 are functions of the location effect estimates that are not in the BH model, they are independent of all $\hat{\beta}_j$ and $\hat{\beta}_{j'}$ which are in the model. Therefore,

$$R = \frac{ng}{n-2}\left(\frac{\sigma^2_{d+} + \sigma^2_{d-}}{s^2_{d+}\sigma^2_{d-} + s^2_{d-}\sigma^2_{d+}}\right) \times \left[(\hat{\beta}_j - \beta_j)^2 - 2\,\frac{\sigma^2_{d+} - \sigma^2_{d-}}{\sigma^2_{d+} + \sigma^2_{d-}}(\hat{\beta}_j - \beta_j)(\hat{\beta}_{j'} - \beta_{j'}) + (\hat{\beta}_{j'} - \beta_{j'})^2\right] \sim F_{2,2g}. \quad (5)$$

Unfortunately, σ^2_{d+} and σ^2_{d-} are not removed. If they were known, $100(1-\alpha)\%$ confidence regions for $(\beta_j, \beta_{j'})$ could be calculated by setting $R \leqslant F_{(1-\alpha),2,2g}$. If we set $\beta_j = \beta_{j'} = 0$ in (5), for a given α, and 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 calculate a statistic by using $\hat{\sigma}^2_{d+} = (n-2)s^2_{d+}/2g$ and $\hat{\sigma}^2_{d-} = (n-2)s^2_{d-}/2g$ from (2) yielding

$$\dot{R} = \frac{ng}{2(n-2)}\left[\left(\frac{1}{s^2_{d+}} + \frac{1}{s^2_{d-}}\right)((\hat{\beta}_j - \beta_j)^2 + (\hat{\beta}_{j'} - \beta_{j'})^2) - 2\left(\frac{1}{s^2_{d+}} - \frac{1}{s^2_{d-}}\right)(\hat{\beta}_{j'} - \beta_{j'})(\hat{\beta}_j - \beta_j)\right]. \quad (6)$$

Due to this substitution of unbiased estimators, $\dot{R}$ will not have an $F_{2,2g}$ distribution. Intuitively, an adjustment should be made in the degrees of freedom. It can be shown that $E(\dot{R}) = g/(g-2)$, the expected value of an $F_{\cdot,g}$ random variable. To see if $\dot{R}$ has an approximate $F_{2,g}$ distribution, simulations were performed using $g = 4, 5, 6, 7$ and $\alpha = 0.10, 0.05, 0.01$. For each condition, 10,000 simulations were performed. (Simulation results are available at *http://www.cba.bgsu.edu/faculty_staff/McGrath/statprob/sims.pdf.*) From these simulations, it is apparent that $\dot{R} \tilde{\sim} F_{2,g}$. Thus we will form approximate $100(1-\alpha)\%$ confidence regions based on (6) by setting $\dot{R} \leqslant F_{(1-\alpha),2,g}$.

Example. As an example, we look at data originally analyzed by Anderson and McLean (1974, pp. 256–259). The experiment was a 2^{5-1} design to study the impact of five factors on an index of "goodness" of asphalt concrete. The data are shown in Table 1. Anderson and McLean used this as an example of how to analyze a $\frac{1}{2}$ fraction with no intention of studying dispersion. As the main effects and two-factor interactions consume all 15 degrees of freedom, they used a previous estimate of 200 for the error mean square. Using this value and performing ANOVA, the F tests are based on 1 and ∞ degrees of freedom. If $\alpha = 0.05$ is used, four effects are found active: AD, AE, BD, and DE. Fitting this location model results in a mean square error of 179.5, reasonably close to the pre-experiment estimate of 200. Note that none of the active effects are main effects.

Table 2 shows the sample variances, D^{BH} statistics, and associated p-values for this four location effect model. Based on D^{BH}, we see that AB and E have mildly significant dispersion effects with p-values of 0.0567 and 0.0424 respectively. However, a limitation of the D^{BH} test is that it is not applicable if multiple dispersion effects are present. In addition, a single dispersion effect inflates the significance level of null dispersion effects. As the D^{BH} tests indicate there may be two dispersion effects, we also apply the recently developed test of McGrath and Lin (2001b). This test is designed for testing multiple dispersion effects, but can only be calculated for certain columns depending on the location model. The results (F^{ML}) are also given in Table 1 along with approximate p-values. Note that using F^{ML}, AB does not appear to have a significant dispersion effect. Unfortunately, E cannot

Table 1
Example effect matrix, responses, and ols location effect estimates

		A	B	C	D	AB	AC	AD	BC	BD	CD	DE	CE	BE	AE	E	y
1	1	−1	−1	−1	−1	1	1	1	1	1	1	−1	−1	−1	−1	1	13
2	1	1	−1	−1	−1	−1	−1	−1	1	1	1	1	1	1	−1	−1	54
3	1	−1	1	−1	−1	−1	1	1	−1	−1	1	1	1	−1	1	−1	44
4	1	1	1	−1	−1	1	−1	−1	−1	−1	1	−1	−1	1	1	1	49
5	1	−1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	1	−1	13
6	1	1	−1	1	−1	−1	1	−1	−1	1	−1	−1	1	−1	1	1	14
7	1	−1	1	1	−1	−1	−1	1	1	−1	−1	−1	1	1	−1	1	18
8	1	1	1	1	−1	1	1	−1	1	−1	−1	1	−1	−1	−1	−1	85
9	1	−1	−1	−1	1	1	1	−1	1	−1	−1	−1	1	1	1	−1	41
10	1	1	−1	−1	1	−1	−1	1	1	−1	−1	1	−1	−1	1	1	73
11	1	−1	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1	−1	1	79
12	1	1	1	−1	1	1	−1	1	−1	1	−1	−1	1	−1	−1	−1	17
13	1	−1	−1	1	1	1	−1	−1	−1	−1	1	1	1	−1	−1	1	82
14	1	1	−1	1	1	−1	1	1	−1	−1	1	−1	−1	1	−1	−1	58
15	1	−1	1	1	1	−1	−1	−1	1	1	1	−1	−1	−1	1	−1	10
16	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	29

$\hat\beta_0=42.4375$ $\hat\beta_A=4.9375$ $\hat\beta_B=-1.0625$ $\hat\beta_C=-3.8125$ $\hat\beta_D=6.1875$ $\hat\beta_{AB}=-1.3125$ $\hat\beta_{AC}=2.9375$ $\hat\beta_{AD}=9.3125$ $\hat\beta_{BC}=-2.0625$ $\hat\beta_{BD}=-13.8125$ $\hat\beta_{CD}=-0.0625$ $\hat\beta_{DE}=14.9375$ $\hat\beta_{CE}=-5.0625$ $\hat\beta_{BE}=0.1875$ $\hat\beta_{AE}=-8.3125$ $\hat\beta_E=2.1875$

Table 2
Concrete experiment dispersion effect statistics

Column	s^2_{d-}	s^2_{d+}	D^{BH}	p-value	F^{ML}	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	0.58	0.682
D	40.79	74.77	1.83	0.6310		
AB	220.14	24.64	0.11	0.0567	0.12	0.134
AC	129.29	60.91	0.47	0.5523		
AD	69.29	208.80	3.01	0.2513	5.56	0.223
BC	60.79	57.34	0.94	0.9629		
BD	179.57	65.21	0.36	0.3502	0.48	0.588
CD	154.07	37.34	0.24	0.2748		
DE	128.29	153.66	1.20	0.8478	2.61	0.483
CE	111.21	34.20	0.31	0.3586		
BE	63.00	181.79	2.89	0.3292	9.59	0.119
AE	145.87	126.44	0.87	0.8792	1.11	0.937
E	5.36	93.05	17.37	0.0424		

be tested using F^{ML}. However, by combining the D^{BH} and F^{ML} findings, we may be reasonably confident that there is at most a single dispersion effect due to E. We make this assumption for the rest of this section.

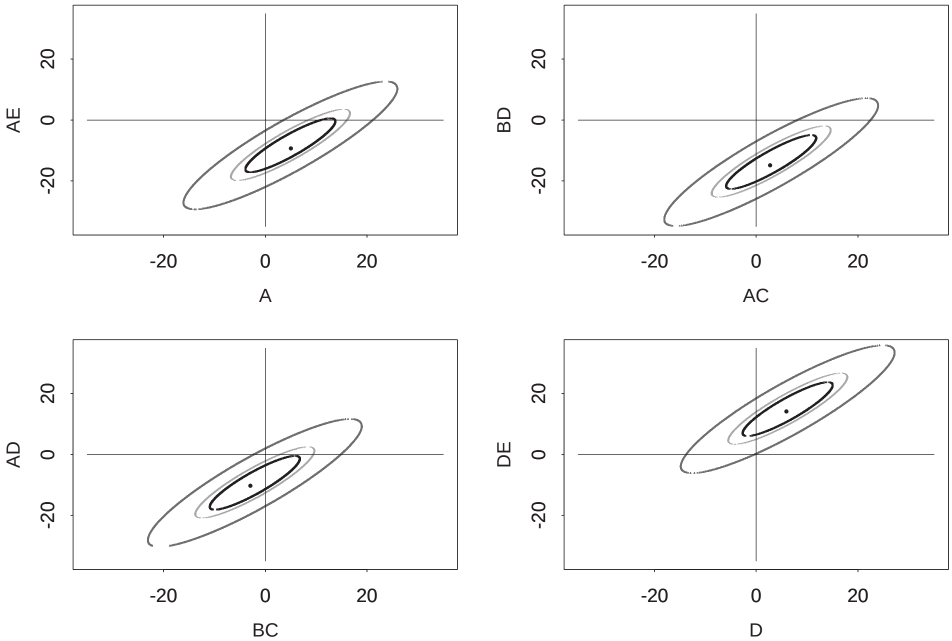

Fig. 1. 90%, 95%, and 99% Confidence regions (E = dispersion effect).

With a dispersion effect in E, $\sigma^2_{E+}/\sigma^2_{E-} = \Delta_E$, we have the following correlation pattern:
Correlation Pattern ($\Delta_E > 1$):

$I : E$	D : **DE**
A : **AE**	$AB : CD$
$B : BE$	AC : **BD**
$C : CE$	**AD** : BC

The notation $AB : CD$, for example, means that $\hat{\beta}_{AB}$ and $\hat{\beta}_{CD}$ are correlated. The "active" effects from the initial analysis are shown in bold. Using (4) with $s^2_{E+} = 93.05$ and $s^2_{E-} = 5.36$, we have $r_E = 87.69/98.41 = 0.89$. Thus, each "active" location effect estimate is highly correlated with an "inactive" estimate.

To study the location effect estimates in pairs, we fit a BH model: $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_E x_{iE} + \hat{\beta}_A x_{iA} + \hat{\beta}_{AE} x_{iAE} + \hat{\beta}_D x_{iD} + \hat{\beta}_{DE} x_{iDE} + \hat{\beta}_{AC} x_{iAC} + \hat{\beta}_{BD} x_{iBD} + \hat{\beta}_{AD} x_{iAD} + \hat{\beta}_{BC} x_{iBC}$. As three pairs are left out of the model, we construct confidence region plots based on (6) with $g = 3$ and $\dot{R} \leqslant F_{(1-\alpha),2,3}$. Fig. 1 shows these plots for the four pairs in the BH model. The smallest ellipse in each plot is the approximate 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 90% region for AE just barely crosses 0 implying the joint region p-value is slightly greater than 0.10.

One drawback of using these p-values is that the joint relationship between paired estimates is not fully considered. 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 joint region p-value is greater than 0.10. In a similar manner, if we believe $AC=0$, then BD is active.

The $D:DE$ region provides another interesting interpretation. DE appears to be active as it is significant at $\alpha=0.05$ regardless of the value of D, but D does not appear to be active as all of the ellipses cross $D=0$. However, if we assume that the DE location effect is the value obtained from the experiment ($\beta_{DE}=14.9375$, an admittedly strong assumption) and slice the ellipse at this value, we find that only the 99% interval crosses $D=0$. Thus, we may conclude that D is an active location effect ($0.01 \leqslant p$-value $\leqslant 0.05$) conditioned on $DE=14.9375$. (Substituting $\hat{\beta}_{DE}=\beta_{DE}$ into (6) and comparing $\dot{R}$ to an $F_{2,3}$ distribution we get a conditional p-value of approximately 0.03.) 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.

4. Summary

In today's modern industry, extremely short product life cycles demand 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 in the previous section.

1. Use a standard procedure, e.g. ANOVA or normal or half-normal plots, to *tentatively* identify active location effects and fit a reduced model.
2. Test for dispersion effects. D^{BH} may be used to test each column, assuming all other columns do not have a dispersion effect. If multiple dispersion effects are suspected, F^{ML} may be used on columns determined by the location model. Use the D^{BH} and F^{ML} results to identify the dispersion effects.
3. Based on step 2,

(a) If no dispersion effects are detected, accept that the effects in (1) are the active location effects and stop.
(b) If a single dispersion effect is considered active, then create confidence region plots for each correlated pair that includes an effect from (1) and identify location effects now believed to be active.
(c) If multiple dispersion effects are identified, additional data appears to be necessary to confidently determine the active location and dispersion effects.

Many techniques view the analysis of location and dispersion effects (to some extent) as separate problems. Another approach, Engel and Huele (1996) and Lee and Nelder (1998), uses generalized linear models. Following Lee and Nelder, we assume a normal distribution with an identity link for the mean model. Squared residuals from this model are the response for the dispersion model using a gamma distribution with a log link. The predicted values from the dispersion model are used as weights for the mean model and the procedure is iterated. However, these weights have no impact on the location estimates of dc pairs when there is a single dispersion effect. Thus, if a BH model is fit, no iteration is necessary and the location and dispersion effect estimates are the same as in our approach.

By studying the correlation among location effect estimates induced by a dispersion effect, we have shown that location effects should not be studied independently in the presence of dispersion. Simulation results (available at *http://www.cba.bgsu.edu/faculty_staff/McGrath/statprob/sims.pdf*) show that while ignoring this correlation does not impact the power of an individual location effect test, it does affect the joint power of pairs of tests. Most results given here are based on the assumption of a single dispersion effect. The extension to multiple dispersion effects has been initially investigated. The complicated correlation structure makes this a very difficult problem and further research is required.

In summary, we recommend that an iterative approach be used beginning by identifying location effects. As shown by McGrath and Lin (2001a), failure to include a pair of location effects in a model and using residuals to study dispersion can create a spurious dispersion effect. 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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