RESPONSE SURFACE ANALYSIS OF EXPERIMENTS
WITH RANDOM BLOCKS

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This article is concerned with the analysis of experiments arranged in blocks where the block effect is considered random. Estimates of the polynomial effects in the model are obtained free of the block effect.

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Response Surface Analysis of Experiments With Random Blocks

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ABSTRACT

This article is concerned with the analysis of experiments arranged in blocks chosen at random. Estimates of the polynomial parameters in the associated response surface model are obtained free of blocks. Tests concerning the polynomial and random block effects are presented. Furthermore, the power of the test for the block effect is obtained using a certain approximation by Hirotsu (1979). A numerical example is given to illustrate the implementation of the proposed analysis.

KEY WORDS: Design moments; Fixed and random effects; Mixed model; Orthogonal blocking; Polynomial and block effects; Response surface model.

1. INTRODUCTION

Model fitting in response surface methodology is usually based on the assumption that the experimental runs are carried out under homogeneous conditions. This, however, may be difficult to achieve in some experiments. For example, the runs may be obtained over a period of time or in batches among which the experimental conditions can vary appreciably. Such an extraneous source of variation should, therefore, be accounted for by introducing a block effect into the response surface model.

Box and Hunter (1957) introduced the concept of orthogonal blocking so that estimates of the polynomial parameters in the model can be obtained free of the block effect. This concept was developed under the presumption that the block effect was fixed, that is, represented by a constant parameter in the model. In this case, "the effect of carrying out a particular trial in one block rather than another is merely to change the expected value of the response by a fixed amount which depends only on the particular blocks involved," as was stated in Box and Hunter (1957, p. 228). Quite often, however, the blocks are selected at random. For example, the blocks can be batches of raw material used in a chemical process. In this case, it would be more appropriate to regard the block effect as random.

In the present article, the analysis of a blocked experiment will be discussed under the assumption that the block effect is random. This analysis does not require that the design blocks orthogonally.

2. SOME PRELIMINARIES

Consider a model of order d (≥ 1) in k input variables, $x_1, x_2, \ldots, x_k$. The experimental runs are arranged in b blocks. The model can therefore be written as

$$\underset{\sim}{y} = \beta_0 \underset{\sim}{1}_n + \underset{\sim}{X}\underset{\sim}{\beta} + \underset{\sim}{Z}\underset{\sim}{\gamma} + \underset{\sim}{\epsilon}, \tag{2.1}$$

where $\underset{\sim}{y}$ is a vector of n observations on the response, β_0 and $\underset{\sim}{\beta} = (\beta_1, \beta_2, \ldots, \beta_p)'$ are unknown parameters associated with the polynomial portion of the model, $\underset{\sim}{\gamma} = (\gamma_1, \gamma_2, \ldots, \gamma_b)'$, where γ_ℓ denotes the effect of the $\ell^{\underline{th}}$ block ($\ell = 1, 2, \ldots, b$), and $\underset{\sim}{\epsilon}$ is a random error vector. The matrices, $\underset{\sim}{X}$ and $\underset{\sim}{Z}$ are known and are of orders $n \times p$ and $n \times b$ and ranks p and b, respectively. The matrix $\underset{\sim}{Z}$ is actually of the form

$$\underset{\sim}{Z} = \bigoplus_{\ell=1}^{b} 1_{n_\ell}, \tag{2.2}$$

where n_ℓ is the number of observation in the $\ell^{\underline{th}}$ block, 1_{n_ℓ} is a vector of ones of order $n_\ell \times 1$ ($\ell = 1, 2, \ldots, b$) and $\oplus$ denotes the direct sum of matrices. In particular, if $d = 2$, that is, the model is of the second order, then (2.1) can be expressed as

$$y_u = \beta_0 + \sum_{i=1}^{k} \theta_i x_{ui} + \sum_{i=1}^{k} \theta_{ii} x_{ui}^2 + \sum_{i<j} \theta_{ij} x_{ui} x_{uj} + \sum_{\ell=1}^{b} \gamma_\ell z_{u\ell} + \epsilon_u, \quad u = 1, 2, \ldots, n, \tag{2.3}$$

where x_{ui} denotes the $u^{\underline{th}}$ level of the $i^{\underline{th}}$ input variable and $z_{u\ell}$ is a "dummy" variable taking the value one if the $u^{\underline{th}}$ trial is carried out in the $\ell^{\underline{th}}$ block and zero otherwise ($i = 1, 2, \ldots, k$; $\ell = 1, 2, \ldots, b$; $u = 1, 2, \ldots, n$).

Box and Hunter's (1957) conditions for orthogonal blocking for model (2.3) are

$$\sum_{u(\ell)} x_{ui} = 0, \quad i = 1, 2, \ldots, k, \tag{2.4}$$

$$\sum_{u(\ell)} x_{ui} x_{uj} = 0, \quad i,j = 1, 2, \ldots, k; \; i \neq j, \tag{2.5}$$

$$\sum_{u(\ell)} x_{ui}^2 = \frac{n_\ell}{n} \sum_{u=1}^{n} x_{ui}^2, \quad i = 1, 2, \ldots, k, \tag{2.6}$$

where $\sum_{u(\ell)}$ denotes summation over the $\ell^{\underline{th}}$ block ($\ell = 1, 2, \ldots, b$). Note that conditions (2.4) and (2.5) presume that the sum of the elements in each column of the design matrix and the sum of the cross products of the elements of each pair of columns are zero (see also Khuri and Cornell 1987, Section 4.7).

If the block effect is fixed, that is, if the γ_ℓ's in (2.3) are unknown constant parameters, then estimates of the polynomial parameters in the model can be obtained in the usual fashion as if the γ_ℓ's do not appear in the model. In general, for a model of order d, an element of the matrix $\underset{\sim}{X}$ in (2.1) can be written as $x_{u1}^{\delta_1} x_{u2}^{\delta_2} \dots x_{uk}^{\delta_k}$, where the δ_i's are nonnegative integers such that $\sum_{i=1}^{k} \delta_i = \delta$ and $1 \leq \delta \leq d$. In order for a design to block orthogonally we must have

$$\sum_{u=1}^{n} x_{u1}^{\delta_1} x_{u2}^{\delta_2} \dots x_{uk}^{\delta_k}(z_{u\ell} - \bar{z}_\ell) = 0, \qquad \ell = 1, 2, \dots, b; \quad \delta = 1, 2, \dots, d. \tag{2.7}$$

It follows that

$$\sum_{u(\ell)} x_{u1}^{\delta_1} x_{u2}^{\delta_2} \dots x_{uk}^{\delta_k} = \frac{n_\ell}{n} \sum_{u=1}^{n} x_{u1}^{\delta_1} x_{u2}^{\delta_2} \dots x_{uk}^{\delta_k}, \qquad \ell = 1, 2, \dots, b; \quad \delta = 1, 2, \dots, d, \tag{2.8}$$

which can be written as

$$\frac{1}{n_\ell} \sum_{u(\ell)} x_{u1}^{\delta_1} x_{u2}^{\delta_2} \dots x_{uk}^{\delta_k} = \left[1^{\delta_1} 2^{\delta_2} \dots k^{\delta_k}\right], \qquad \ell = 1, 2, \dots, b; \quad \delta = 1, 2, \dots, d, \tag{2.8}$$

where

$$\left[1^{\delta_1} 2^{\delta_2} \dots k^{\delta_k}\right] = \frac{1}{n} \sum_{u=1}^{n} x_{u1}^{\delta_1} x_{u2}^{\delta_2} \dots x_{uk}^{\delta_k} \tag{2.9}$$

is a design moment of order $\delta = \sum_{i=1}^{k} \delta_i$. In particular, if the odd design moments are zero (a design moment is odd if at least one δ_i, i = 1, 2,..., k, is an odd integer), then condition (2.8) requires that

$$\sum_{u(\ell)} x_{u1}^{\delta_1} x_{u2}^{\delta_2} \dots x_{uk}^{\delta_k} = 0, \qquad \ell = 1, 2, \dots, b. \tag{2.10}$$

Condition (2.8) is therefore a generalization of conditions (2.4) – (2.6). It can be noted that the quantity on the left side of (2.8) does not depend on subscript ℓ and is thus invariant with respect to blocks if the design blocks orthogonally. In this case, if $\underset{\sim}{X}_\ell$ denotes the portion of the matrix $\underset{\sim}{X}$ corresponding to block ℓ (= 1, 2,..., b), then from (2.8), the $1 \times p$ vector,

$$\xi' = \frac{1}{n_\ell} 1'_{n_\ell} X_\ell, \qquad (2.11)$$

does not depend on subscript ℓ and is therefore the same for all the blocks.

3. THE ANALYSIS OF EXPERIMENTS WITH RANDOM BLOCKS

Let us assume that the block effect in (2.1) is random such that γ is distributed as $N\left(0, \sigma^2_\gamma I_b\right)$ independently of ϵ, which has the normal distribution $N\left(0, \sigma^2_\epsilon I_n\right)$. Model (2.1) is therefore a mixed model since β is a fixed parameter vector. In this case, the expected value and variance-covariance matrix of y are

$$E(y) = \beta_0 1_n + X\beta, \qquad (3.1)$$

$$Var(y) = \sigma^2_\gamma ZZ' + \sigma^2_\epsilon I_n \qquad (3.2)$$

$$= \sigma^2_\gamma \bigoplus_{\ell=1}^{b} J_{n_\ell} + \sigma^2_\epsilon I_n, \qquad (3.3)$$

where J_{n_ℓ} is the matrix of ones of order $n_\ell \times n_\ell$. The eigenvalues of J_{n_ℓ} are n_ℓ and 0 of multiplicity $n_\ell - 1$ ($\ell = 1, 2, \ldots, b$). By the Spectral Decomposition Theorem, J_{n_ℓ} can be expressed as

$$J_{n_\ell} = P_\ell \Lambda_\ell P'_\ell, \quad \ell = 1, 2, \ldots, b, \qquad (3.4)$$

where Λ_ℓ is the diagonal matrix, diag(n_ℓ, 0) with 0 being a zero matrix of order $(n_\ell-1)\times(n_\ell-1)$, and P_ℓ is an orthogonal matrix of the form

$$P_\ell = \left[\frac{1_{n_\ell}}{\sqrt{n_\ell}} : \; Q_\ell\right], \quad \ell = 1, 2, \ldots, b. \qquad (3.5)$$

Note that for $\ell = 1, 2, \ldots, b$,

$$1'_{n_\ell} Q_\ell = 0 \qquad (3.6)$$

$$Q_\ell' Q_\ell = I_{n_\ell - 1} \tag{3.7}$$

$$Q_\ell Q_\ell' = I_{n_\ell} - J_{n_\ell} / n_\ell . \tag{3.8}$$

Formula (3.3) can then be written as

$$\text{Var}(y) = \sigma_\gamma^2 P \Lambda P' + \sigma_\epsilon^2 I_n, \tag{3.9}$$

where

$$P = \bigoplus_{\ell=1}^{b} P_\ell \tag{3.10}$$

$$\Lambda = \bigoplus_{\ell=1}^{b} \Lambda_\ell . \tag{3.11}$$

Now, let u be defined as

$$u = P' y . \tag{3.12}$$

Then,

$$E(u) = P' \left(\beta_0 1_n + X \beta \right)$$

$$\text{Var}(u) = \sigma_\gamma^2 \bigoplus_{\ell=1}^{b} \Lambda_\ell + \sigma_\epsilon^2 I_n .$$

We note that the elements of u are independent. By rearranging these elements, it is possible to partition u into u_1 and u_2 of orders $b \times 1$ and $(n-b) \times 1$, respectively, such that

$$u_1 = \left[\bigoplus_{\ell=1}^{b} \frac{1_{n_\ell}'}{\sqrt{n_\ell}} \right] y \tag{3.13}$$

$$u_2 = \left[\bigoplus_{\ell=1}^{b} Q_\ell' \right] y . \tag{3.14}$$

From (3.1) and (3.3), the expected value and variance-covariance matrix of u_2 are

$$E(u_2) = \left[\bigoplus_{\ell=1}^{b} Q_\ell' \right] X \beta \tag{3.15}$$

$$\text{Var}(u_2) = \sigma_\epsilon^2 I_{n-b} . \tag{3.16}$$

3.1 The Analysis Concerning the Polynomial Effects

From (3.15) and (3.16), the vector $\underline{u}_2$ can be represented by the model

$$\underline{u}_2 = \underline{T}\underline{\beta} + \underline{\eta}, \tag{3.17}$$

where

$$\underline{T} = \left[\bigoplus_{\ell=1}^{b} \underline{Q}'_\ell \right] \underline{X}, \tag{3.18}$$

and $\underline{\eta}$ is a random vector distributed as $N\left(\underline{0},\ \sigma_\epsilon^2 \underline{I}_{n-b}\right)$. Since $\underline{X}$ is of full column rank equal to p, then $\underline{T}$, which is of order $(n-b)\times p$, is also of rank p provided that $n-b>p$ and the matrix $\underline{S} = [\underline{X}:\ \underline{Z}]$ is of full column rank (see Appendix A). The least squares estimator of $\underline{\beta}$ is therefore given by

$$\hat{\underline{\beta}} = \left(\underline{T}'\underline{T}\right)^{-1} \underline{T}'\underline{u}_2,$$

which can also be written as

$$\hat{\underline{\beta}} = \left(\underline{X}'\underline{W}\underline{X}\right)^{-1} \underline{X}'\underline{W}\underline{y}, \tag{3.19}$$

where

$$\underline{W} = \underline{I}_n - \bigoplus_{\ell=1}^{b} \frac{1}{n_\ell} \underline{J}_{n_\ell}. \tag{3.20}$$

Formula (3.20) is true because

$$\bigoplus_{\ell=1}^{b} \left(\underline{Q}_\ell \underline{Q}'_\ell\right) = \bigoplus_{\ell=1}^{b} \left(\underline{I}_{n_\ell} - \frac{\underline{J}_{n_\ell}}{n_\ell}\right)$$

as can be seen from (3.8). In particular, if the design blocks orthogonally, then $\hat{\underline{\beta}}$ can be shown to be identical to the least-squares estimate of $\underline{\beta}$ obtained for model (2.1) when $\underline{\gamma}$ is fixed. The proof of this assertion is given in Appendix B.

The regression and residual sum of squares for model (3.17) are

$$SS_{Reg} = \underset{\sim}{u}_2'\underset{\sim}{T}\left(\underset{\sim}{T}'\underset{\sim}{T}\right)^{-1}\underset{\sim}{T}'\underset{\sim}{u}_2 \tag{3.21}$$

$$= \underset{\sim}{y}'\underset{\sim}{W}\underset{\sim}{X}\left(\underset{\sim}{X}'\underset{\sim}{W}\underset{\sim}{X}\right)^{-1}\underset{\sim}{X}'\underset{\sim}{W}\underset{\sim}{y}, \tag{3.22}$$

$$SS_E = \underset{\sim}{u}_2'\underset{\sim}{u}_2 - SS_{Reg} \tag{3.23}$$

$$= \underset{\sim}{y}'\left[\underset{\sim}{W} - \underset{\sim}{W}\underset{\sim}{X}\left(\underset{\sim}{X}'\underset{\sim}{W}\underset{\sim}{X}\right)^{-1}\underset{\sim}{X}'\underset{\sim}{W}\right]\underset{\sim}{y}. \tag{3.24}$$

It is interesting to note that SS_{Reg} is in fact equal to $R\left(\underset{\sim}{\beta} \mid \beta_0, \underset{\sim}{\gamma}\right)$, the increase in the regression sum of squares due to adding $\underset{\sim}{\beta}$ to a model that contains the intercept β_0 and the block effect $\underset{\sim}{\gamma}$. This can be clearly seen from the fact that

$$\begin{aligned} \underset{\sim}{y}'\underset{\sim}{y} &= \underset{\sim}{u}'\underset{\sim}{u} \\ &= \underset{\sim}{u}_1'\underset{\sim}{u}_1 + \underset{\sim}{u}_2'\underset{\sim}{u}_2 \\ &= \sum_{\ell=1}^{b} \frac{\tau_\ell^2}{n_\ell} + SS_{Reg} + SS_E, \end{aligned}$$

where τ_ℓ is the total for block ℓ (= 1, 2,..., b). Hence, the total sum of squares, SS_{Tot}, for model (2.1) is

$$SS_{Tot} = \underset{\sim}{y}'\underset{\sim}{y} - \frac{\left(\sum_{\ell=1}^{b} \tau_\ell\right)^2}{n} \tag{3.25}$$

$$= \sum_{\ell=1}^{b} \frac{\tau_\ell^2}{n_\ell} - \frac{\left(\sum_{\ell=1}^{b} \tau_\ell\right)^2}{n} + SS_{Reg} + SS_E. \tag{3.26}$$

But,

$$\sum_{\ell=1}^{b} \frac{\tau_\ell^2}{n_\ell} - \frac{\left(\sum_{\ell=1}^{b} \tau_\ell\right)^2}{n} = R\left(\underset{\sim}{\gamma} \mid \beta_0\right) \tag{3.27}$$

is the increase in the regression sum of squares due to adding $\underset{\sim}{\gamma}$ to a model that only contains the intercept. This is the usual sum of squares for blocks, SS_{Block}, used in the analysis of orthogonally blocked experiments with fixed blocks. From (3.26) and (3.27) we then have

$$SS_{Tot} = R\left(\underset{\sim}{\gamma} \mid \beta_0\right) + SS_{Reg} + SS_E, \tag{3.28}$$

which indicates that $SS_{Reg} = R\left(\underset{\sim}{\beta} \mid \beta_0, \underset{\sim}{\gamma}\right)$. In particular, if the design blocks orthogonally, then $SS_{Reg} = R\left(\underset{\sim}{\beta} \mid \beta_0\right)$, which is the regression sum of squares for the polynomial effects obtained by ignoring the block effect in model (2.1).

When replicate observations on the response are available within the blocks, the residual sum of squares can be partitioned into a lack of fit sum of squares, SS_{LOF}, and a pure error sum of squares, SS_{PE}. The latter is obtained by pooling the pure error sums of squares from the blocks. Tests concerning the polynomial effects can then proceed using SS_{PE} as the error term in the denominators of the F test statistics.

3.2 The Analysis Concerning the Block Effect

The sum of squares for blocks given in (3.27), namely $R\left(\underset{\sim}{\gamma} \mid \beta_0\right)$, is not appropriate to test the hypothesis

$$H_0: \ \sigma_\gamma^2 = 0 \tag{3.29}$$

versus the alternative hypothesis

$$H_a: \ \sigma_\gamma^2 \neq 0,$$

if the design does not block orthogonally. This is because the expected value of $R\left(\underset{\sim}{\gamma} \mid \beta_0\right)$ is not free of the fixed polynomial effects. Since model (2.1) is basically a mixed model, a more appropriate sum of squares to use to test the block effect is $R\left(\underset{\sim}{\gamma} \mid \beta_0, \underset{\sim}{\beta}\right)$, which represents the increase in the regression sum of squares due to adding $\underset{\sim}{\gamma}$ to a model that contains the intercept β_0 and the vector of polynomial parameters, $\underset{\sim}{\beta}$. The expected value of the latter sum of squares is free of all fixed polynomial effects (see, for example, Searle 1971, Chapter 10). More specifically,

$$E\left[R\left(\underset{\sim}{\gamma} \mid \beta_0, \underset{\sim}{\beta}\right)\right] = \sigma_\gamma^2 \operatorname{tr}\left\{\underset{\sim}{Z}'\left[\underset{\sim}{I}_n - \tilde{\underset{\sim}{X}}(\tilde{\underset{\sim}{X}}'\tilde{\underset{\sim}{X}})^{-1}\tilde{\underset{\sim}{X}}'\right]\underset{\sim}{Z}\right\} + (b-1)\sigma_\epsilon^2, \tag{3.30}$$

where $\tilde{\underset{\sim}{X}} = [\underset{\sim}{1}_n : \underset{\sim}{X}]$. Formula (3.30) follows from applying formula (79) in Searle (1971, p. 445). Furthermore, under H_0, $R\left(\underset{\sim}{\gamma} \mid \beta_0, \underset{\sim}{\beta}\right)/\sigma_\epsilon^2$ has the chi-square distribution with b−1 degrees of freedom. Thus, an appropriate test statistic for the hypothesis H_0 is

$$F = \frac{R\left(\underset{\sim}{\gamma} \mid \beta_0, \underset{\sim}{\beta}\right)}{(b-1)MS_{PE}}, \tag{3.31}$$

which under H_0 has the F distribution with b−1 and ν degrees of freedom, where ν and MS_{PE} are the number of degrees of freedom and mean square for the pure error, respectively.

3.2.1 The Power of the Test

Under the alternative hypothesis H_a, $R\left(\underset{\sim}{\gamma} \mid \beta_0, \underset{\sim}{\beta}\right)/\sigma_\epsilon^2$ does not have the chi-square distribution. Instead, $R\left(\underset{\sim}{\gamma} \mid \beta_0, \underset{\sim}{\beta}\right)$ is distributed as $\sum_{i=1}^{n} \lambda_i V_i$, where the V_i's are independent chi-square variates with one degree of freedom each, and the λ_i's are the eigenvalues of the matrix

$$\underset{\sim}{\Omega} = \left(\sigma_\gamma^2 \underset{\sim}{Z}\underset{\sim}{Z}' + \sigma_\epsilon^2 \underset{\sim}{I}_n\right)\left[\underset{\sim}{S}\left(\underset{\sim}{S}'\underset{\sim}{S}\right)^{-1}\underset{\sim}{S}' - \tilde{\underset{\sim}{X}}\left(\tilde{\underset{\sim}{X}}'\tilde{\underset{\sim}{X}}\right)^{-1}\tilde{\underset{\sim}{X}}'\right], \tag{3.32}$$

where $\underset{\sim}{S} = [\underset{\sim}{X} : \underset{\sim}{Z}]$. See Johnson and Kotz (1970, p. 151). This fact can be used to obtain approximate power values for the test by using Hirotsu's (1979, pp. 578-579) approximation (see also Khuri 1987, pp. 308-310). More specifically, the power can be computed using the approximation

$$P\left(F \ge F_{\alpha, b-1, \nu} \mid H_a\right) \approx P\left(F_{f,\nu} \ge h\right) + \left[\Delta \Big/ \left\{3(f+2)(f+4)B\left(\tfrac{f}{2}, \tfrac{\nu}{2}\right)\right\}\right]\left(1 + \tfrac{f\,h}{\nu}\right)^{-(f+\nu)/2} \times$$

$$\left(\tfrac{f\,h}{\nu}\right)^{f/2} \times \left[(f+2)(f+4) + \frac{2(f+\nu)(f+4)}{1+\nu/(f\,h)} + \frac{(f+\nu+2)(f+\nu)}{\{1+\nu/(f\,h)\}^2}\right], \tag{3.33}$$

where

$F_{b-1,\nu}$ denotes the F distribution with b−1 and ν degrees of freedom and $F_{\alpha,b-1,\nu}$ is its upper $\alpha 100\%$ point, $B\left(\frac{f}{2}, \frac{\nu}{2}\right)$ denotes the beta function with parameters f/2 and $\nu/2$,

$$h = \sigma_\epsilon^2 (b - 1) F_{\alpha,b-1,\nu} \Big/ \mathrm{tr}(\Omega),$$

$$f = \left[\mathrm{tr}(\Omega)\right]^2 \Big/ \mathrm{tr}(\Omega^2),$$

$$\Delta = \frac{\mathrm{tr}(\Omega)\mathrm{tr}(\Omega^3)}{\left[\mathrm{tr}(\Omega^2)\right]^2} - 1.$$

Formula (3.33) was derived from formula (3.5) in Khuri (1987, p. 309).

4. A NUMERICAL EXAMPLE

The yield, y, of a chemical process was measured at various levels of temperature, catalyst concentration, and reaction time. The coded levels of these input variables are denoted by x_1, x_2, and x_3, respectively. The mean response was represented by a second-order model of the form

$$E(y) = \beta_0 + \sum_{i=1}^{3} \theta_i x_i + \theta_{12} x_1 x_2 + \theta_{13} x_1 x_3 + \theta_{23} x_2 x_3 + \sum_{i=1}^{3} \theta_{ii} x_i^2. \quad (4.1)$$

Three batches of raw material were randomly selected and used in this experiment. Each batch was only large enough to permit a maximum of eight runs to be made. Some variation was suspected to exist among the batches since they were received at different times. The batches were therefore considered as blocks. The design used was a central composite design consisting of the three blocks shown in Table 1. This design is rotatable since α, the value of the axial distance, is equal to 1.682, which is the fourth root of 8, the number of factorial points (see, for example, Khuri and Cornell 1987, p. 118). The design, however, does not block orthogonally since an α value of 1.512 would be needed for this purpose as can be verified by invoking formula (2.6). The observed response values are also given in Table 1.

Using formula (3.19), the least-squares estimate of $\underset{\sim}{\beta}$, the vector of nine coefficients in formula (4.1), is given by

$$\hat{\underset{\sim}{\beta}} = (1.496,\ 1.145,\ .382,\ -2.734,\ -1.701,\ -1.037,\ 1.860,\ -.958,\ 1.409)'.$$

The regression and residual sum of squares defined in (3.22) and (3.24), respectively, have the values, $SS_{Reg} = 240.695$, $SS_E = 7.4792$ with 9 and 10 degrees of freedom, respectively. The pooled pure error sum of squares from the replicates at the center point in each of the three blocks is equal to $SS_{PE} = 2.0127$ with 5 degrees of freedom. Hence, the lack of fit sum of squares is $SS_{LOF} = 5.4665$ with 5 degrees of freedom. Consequently, the lack of fit test statistic has the value

$$F = \frac{5.4665/5}{2.0127/5} = 2.72,$$

with a corresponding p-value of .148 (see also Table 2).

The linear and quadratic effects associated with the three input variables are displayed in Table 2. Their sums of squares form a partitioning of $R\left(\underset{\sim}{\beta} \mid \beta_0, \underset{\sim}{\gamma}\right)$, which is equal to $SS_{Reg} = 240.695$. On the other hand, the sum of squares for blocks adjusted for the polynomial effects, that is, $R\left(\underset{\sim}{\gamma} \mid \beta_0, \underset{\sim}{\beta}\right)$ is equal to 121.4246. Hence, the test statistic given in (3.31) for the hypothesis H_0 in (3.29) concerning the block effect has the value

$$F = \frac{121.4246}{2(2.0127/5)} = 150.82,$$

which is highly significant (the p-value is .000034).

5. CONCLUDING REMARKS

The conditions for orthogonal blocking impose certain constraints on the settings of the input variables. Some of these settings may not be feasible from the experimental point of view. The analysis described in this article can be applied whether the design blocks orthogonally or not. It can be conveniently carried out by using standard statistical computer packages such as SAS. This provides the researcher with more flexibility in the choice of design.

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APPENDIX A: THE RANK OF THE MATRIX $\underset{\sim}{T}$ DEFINED IN FORMULA (3.18)

Let $r(\cdot)$ denote the rank of a matrix. Then

$$\begin{aligned} r(\underset{\sim}{T}) &= r(\underset{\sim}{T}'\underset{\sim}{T}) \\ &= r\left\{\underset{\sim}{X}'\left[\bigoplus_{\ell=1}^{b} \underset{\sim}{Q}_\ell \underset{\sim}{Q}_\ell'\right]\underset{\sim}{X}\right\} \\ &= r\left\{\underset{\sim}{X}'\left[\bigoplus_{\ell=1}^{b}\left(\underset{\sim}{I}_{n_\ell} - \frac{\underset{\sim}{J}_{n_\ell}}{n_\ell}\right)\right]\underset{\sim}{X}\right\}, \text{ by (3.8),} \\ &= r\left\{\left[\bigoplus_{\ell=1}^{b}\left(\underset{\sim}{I}_{n_\ell} - \frac{\underset{\sim}{J}_{n_\ell}}{n_\ell}\right)\right]\underset{\sim}{X}\right\}. \end{aligned}$$

Now, suppose that $\left[\bigoplus_{\ell=1}^{b}\left(\underset{\sim}{I}_{n_\ell} - \underset{\sim}{J}_{n_\ell}/n_\ell\right)\right]\underset{\sim}{X}$ is not of full column rank. Then there exists $\underset{\sim}{a} \neq \underset{\sim}{0}$ such that $\left[\bigoplus_{\ell=1}^{b}\left(\underset{\sim}{I}_{n_\ell} - \underset{\sim}{J}_{n_\ell}/n_\ell\right)\right]\underset{\sim}{X}\underset{\sim}{a} = \underset{\sim}{0}$. It follows that

$$\underset{\sim}{X}\underset{\sim}{a} = \left[\bigoplus_{\ell=1}^{b}\left(\underset{\sim}{J}_{n_\ell}/n_\ell\right)\right]\underset{\sim}{X}\underset{\sim}{a}. \tag{A.1}$$

The matrix $\underset{\sim}{X}$ can be partitioned as $\underset{\sim}{X} = \left[\underset{\sim}{X}_1' : \underset{\sim}{X}_2' : \ldots : \underset{\sim}{X}_b'\right]'$, where $\underset{\sim}{X}_\ell$ corresponds to block ℓ

(= 1, 2,..., b). From (A.1) we then get

$$\underset{\sim}{X}\underset{\sim}{a} = \left[\bigoplus_{\ell=1}^{b} \underset{\sim}{1}_{n_\ell}\right]\underset{\sim}{\zeta}$$

$$= \underset{\sim}{Z}\underset{\sim}{\zeta}, \text{ by (2.2)}, \tag{A.2}$$

where $\underset{\sim}{\zeta} = \left(\zeta_1, \zeta_2, \ldots, \zeta_b\right)'$ and ζ_ℓ is defined by

$$\zeta_\ell = \left(\underset{\sim}{1}'_{n_\ell}\underset{\sim}{X}_\ell / n_\ell\right)\underset{\sim}{a}, \qquad \ell = 1, 2, \ldots, b. \tag{A.3}$$

From (A.2) we conclude that

$$\underset{\sim}{S}\left[\underset{\sim}{a}': -\underset{\sim}{\zeta}'\right]' = \underset{\sim}{0}, \tag{A.4}$$

where $\underset{\sim}{S} = [\underset{\sim}{X}: \underset{\sim}{Z}]$. This means that the columns of $\underset{\sim}{S}$ are linearly dependent, which contradicts the assumption that it is of full column rank. Hence, the columns of $\underset{\sim}{T}$ must be linearly independent and its rank equal to p, the rank of $\underset{\sim}{X}$.

APPENDIX B: FORMULA (3.19) UNDER ORTHOGONAL BLOCKING

Consider formulas (3.19) and (3.20). If the design blocks orthogonally, then by (2.11) $\hat{\underset{\sim}{\beta}}$ can be written as

$$\hat{\underset{\sim}{\beta}} = \left(\underset{\sim}{X}'\underset{\sim}{X} - n\underset{\sim}{\xi}\underset{\sim}{\xi}'\right)^{-1}\left[\underset{\sim}{X}'\underset{\sim}{y} - \left(\sum_{u=1}^{n} y_u\right)\underset{\sim}{\xi}\right]$$

$$= \left(\underset{\sim}{X}'\underset{\sim}{X}\right)^{-1}\left[\underset{\sim}{I}_p + \frac{n\underset{\sim}{\xi}\underset{\sim}{\xi}'\left(\underset{\sim}{X}'\underset{\sim}{X}\right)^{-1}}{1-d}\right]\left[\underset{\sim}{X}'\underset{\sim}{y} - \left(\sum_{u=1}^{n} y_u\right)\underset{\sim}{\xi}\right]$$

$$= \left(\underset{\sim}{X}'\underset{\sim}{X}\right)^{-1}\left[\underset{\sim}{X}'\underset{\sim}{y} + \frac{n\underset{\sim}{\xi}\underset{\sim}{\xi}'\left(\underset{\sim}{X}'\underset{\sim}{X}\right)^{-1}\underset{\sim}{X}'\underset{\sim}{y} - \left(\sum_{u=1}^{n} y_u\right)\underset{\sim}{\xi}}{1-d}\right], \tag{B.1}$$

where $d = n\underset{\sim}{\xi}'\left(\underset{\sim}{X}'\underset{\sim}{X}\right)^{-1}\underset{\sim}{\xi}$.

Now, let $\hat{\underset{\sim}{\beta}}_r$ denote the least-squares estimate of $\underset{\sim}{\beta}$ when $\underset{\sim}{\gamma}$ is ignored in model (2.1). This is the usual least-squares estimate obtained under orthogonal blocking when the block effect is fixed. In this case $\hat{\underset{\sim}{\beta}}_r$ can be determined from the equation

$$\begin{bmatrix} \hat{\beta}_0 \\ \hat{\underset{\sim}{\beta}}_r \end{bmatrix} = \begin{bmatrix} n & \underset{\sim}{1}_n'\underset{\sim}{X} \\ \underset{\sim}{X}'\underset{\sim}{1}_n & \underset{\sim}{X}'\underset{\sim}{X} \end{bmatrix}^{-1} \begin{bmatrix} \underset{\sim}{1}_n' \\ \underset{\sim}{X}' \end{bmatrix} \underset{\sim}{y}.$$

Hence,

$$\hat{\underset{\sim}{\beta}}_r = \left(\underset{\sim}{X}'\underset{\sim}{X}\right)^{-1}\underset{\sim}{X}'\underset{\sim}{y} + \frac{n\left(\underset{\sim}{X}'\underset{\sim}{X}\right)^{-1}\underset{\sim}{\xi}\underset{\sim}{\xi}'\left(\underset{\sim}{X}'\underset{\sim}{X}\right)^{-1}\underset{\sim}{X}'\underset{\sim}{y} - \left(\sum_{u=1}^{n} y_u\right)\left(\underset{\sim}{X}'\underset{\sim}{X}\right)^{-1}\underset{\sim}{\xi}}{1-d},$$

which is identical to $\hat{\underset{\sim}{\beta}}$ in (B.1).

REFERENCES

Box, G.E.P., and Hunter, J.S. (1957), "Multi-Factor Experimental Designs for Exploring Response Surfaces," Annals of Mathematical Statistics, 28, 195-241.

Hirotsu, C. (1979), "An F Approximation and its Application," Biometrika, 66, 577-584.

Johnson, N.L., and Kotz, S. (1970), Continuous Univariate Distributions—2, New York: Wiley.

Khuri, A.I. (1987), "An Exact Test for the Nesting Effect's Variance Component in an Unbalanced Random Two-Fold Nested Model," Statistics and Probability Letters, 5, 305-311.

Khuri, A.I., and Cornell, J.A. (1987), Response Surfaces, New York: Dekker.

Searle, S.R. (1971), Linear Models, New York: Wiley.

Table 1. The Design Settings and Response Values for the Numerical Example

Uncoded Variables			Coded Variables			Response
Temperature (°C)	Concentration (%)	Time (h)	x_1	x_2	x_3	y (oz)
170	20	3	1	−1	−1	75.505
150	26	3	−1	1	−1	72.623
150	20	7	−1	−1	1	69.377
170	26	7	1	1	1	70.024
160	23	5	0	0	0	70.171
160	23	5	0	0	0	69.574
160	23	5	0	0	0	70.179
150	20	3	−1	−1	−1	57.202
170	26	3	1	1	−1	68.801
170	20	7	1	−1	1	69.686
150	26	7	−1	1	1	69.460
160	23	5	0	0	0	63.850
160	23	5	0	0	0	63.787
160	23	5	0	0	0	65.136
176.82	23	5	1.682	0	0	75.300
143.18	23	5	−1.682	0	0	72.281
160	28.05	5	0	1.682	0	67.752
160	17.95	5	0	−1.682	0	63.885
160	23	8.36	0	0	1.682	72.752
160	23	1.64	0	0	−1.682	72.278
160	23	5	0	0	0	67.146
160	23	5	0	0	0	68.253

Table 2. Analysis of Variance Table for the Numerical Example

Source	Degrees of Freedom	Sum of Squares (Type I)	F Value	p-Value
Blocks	2	126.592		
Linear regression				
x_1	1	30.566	75.93	.00033
x_2	1	17.915	44.50	.00114
x_3	1	1.900	4.94	.07688
Quadratic regression				
x_1x_2	1	59.787	148.52	.00007
x_1x_3	1	23.147	57.50	.00063
x_2x_3	1	8.603	21.37	.00572
x_1^2	1	52.429	140.46	.00008
x_2^2	1	15.798	33.95	.00210
x_3^2	1	30.550	83.80	.00026
Residual				
Lack of fit	5	5.4665	2.72	.148
Pure error	5	2.0127		