PROTECTING MAIN EFFECT MODELS AGAINST TWO-FACTOR INTERACTION BIAS IN FRACTIONS OF 2^r FACTORIAL DESIGNS

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Institute of Statistics
Mimeograph Series No. 929
June, 1974

(Thesis revised for Publication)

PROTECTING MAIN EFFECT MODELS AGAINST TWO-FACTOR INTERACTION BIAS IN FRACTIONS OF 2^r FACTORIAL DESIGNS

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ABSTRACT

Minimum bias estimation is applied to the classical experimental design situation where the factors are qualitative. A true experimental model for a 2^r factorial design which consists of the mean, main effects, and two-factor interactions is approximated by a function containing only the estimated mean and the estimated main effects. For this true model and approximating function, criteria are developed which indicate when regular and irregular fractional factorial designs allow the bias due to the presence of two-factor interactions to be minimized. Regular fractions are constructed by specifying an identity relation while irregular fractions are constructed by combining regular fractions. For regular fractions to allow the existence of the minimum bias estimator, it is necessary and sufficient that they be resolution IV designs with at least 2r design points. Resolution IV regular fractions satisfy the Box-Draper condition in which case the minimum bias estimator becomes the ordinary least squares estimator. Irregular fractions that allow minimum bias estimators may be constructed by combining regular fractions which have resolution less than IV. Irregular fractions that are constructed in this manner are cataloged for $3(2^{r-2})$ and $3(2^{r-3})$ designs when r = 3, 4, 5, and 6. For seven or more factors, irregular fractions for $3(2^{r-2})$ and $3(2^{r-3})$ designs that allow minimum bias estimators and satisfy the Box-Draper condition, can be constructed by combining the resolution IV regular fractions of 2^{r-2} and 2^{r-3} designs.

1. INTRODUCTION

When a true model; $\eta = \underline{x}_1'\underline{\beta}_1 + \underline{x}_2'\underline{\beta}_2$ is approximated by $\hat{y} = \underline{x}_1'\underline{b}_1$ over a region of experimentation $(\underline{x}_1' \vdots \underline{x}_2') \in R$, discrepancies between the approximate and true response stem from both the sampling error (i.e., variance error), and the inadequacy of the approximating function to represent exactly the true response model (i.e., bias error). In 1959, Box and Draper, (BD), [3] considered both the variance error and the bias error by studying designs that minimize the mean square error (MSE) of $\hat{y}$ averaged over the region R. Because the contribution of the bias term dominates the contribution of the variance term in the average MSE, Box and Draper proposed that an experimenter (1) estimate $\underline{\beta}_1$ by ordinary least squares methods (OLS), and (2) find an experimental design $R^* \subset R$ which minimizes the bias term. If $X^* = (X_1^* \vdots X_2^*)$ is a matrix of the n-design points of R^*, a necessary and sufficient condition for a design to minimize the bias term is the BD condition: $H_{11}^{-1}H_{12} = M_{11}^{-1}M_{12}$ where the regional moments are $H_{ij} = \Omega\int_R \underline{x}_i\underline{x}_j' d\underline{x}$ with $\Omega^{-1} = \int_R d\underline{x}$ and the design moments are $M_{ij} = n^{-1}X_i^{*\prime}X_j^*$ for i and j = 1, 2.

In 1969, Karson, Manson and Hader, (KMH), [8] were able to find smaller average MSE than is obtained using the BD method by proposing that an experimenter (1) estimate $\underline{\beta}_1$ so as to minimizes the bias term, and (2) find an experimental design R^* which minimizes the variance term. A necessary and sufficient condition for the existence of a minimum bias estimator (MBE) is that the experimental design R^* allow estimation of the linear combination of parameters $G\underline{\beta} = [I \vdots H_{11}^{-1}H_{12}][\underline{\beta}_1' \vdots \underline{\beta}_2']'$. The KMH method has been applied to the polynomial model [8], the exponential model [12], the mixture problem [11], and rational functions [4]. In each of these applications, the approximating function is a low order polynomial with variables defined over a continuous space.

This paper is concerned with applying the KMH method to the classical experimental design situation where the factors each have a finite number of levels. For this situation, the region of experimentation R consists of a finite number of lattice points.

2. DERIVATION OF THE ESTIMATOR

Let the region of experimentation R be the set of points representing all combinations of the levels of the experimental variables. R is a set of m lattice points. The true model over R is expressed as: $\underline{\eta} = X_1\underline{\beta}_1 + X_2\underline{\beta}_2 = X\underline{\beta}$, where $\underline{\eta} = [\eta(\underline{x}_1), \ldots, \eta(\underline{x}_m)]'$; $\underline{x}_i = [\underline{x}'_{i1} \vdots \underline{x}'_{i2}]'$, $i = 1, 2, \ldots, m$; $X_1 = [\underline{x}_{11}, \ldots, \underline{x}_{m1}]'$, a matrix of full column rank p; $X_2 = [\underline{x}_{12}, \ldots, \underline{x}_{m2}]'$; $X = [X_1 \vdots X_2]$, $\underline{\beta}_1$ is a $p \times 1$ vector of parameters; $\underline{\beta}_2$ is a $k \times 1$ vector of parameters and $\underline{\beta} = [\underline{\beta}'_1 \vdots \underline{\beta}'_2]'$. To facilitate the derivation of the MBE, the matrix X_1 is assumed to have full column rank (X_1 can always be reparameterized to full column rank).

Let the estimates of the p parameters in $\underline{\beta}_1$ be the terms in $\underline{b}_1$ of the approximating function:

$$\hat{\underline{y}} = X_1\underline{b}_1 .$$

A linear transformation of the $n \times 1$ vector of observations $\underline{y}^*$ is chosen to estimate $\underline{\beta}_1$ (i.e., $\underline{b}_1 = T'\underline{y}^*$), where an asterisk (*) indicates the vectors which are associated with the experimental design R^*.

If the observed response at the i^{th} point in R is $Y(\underline{x}_i) = \eta(\underline{x}_i) + e_i$ where $i = 1, 2, \ldots, m$ and the random variable e_i has $E(e_i) = 0$, $E(e_i^2) = \sigma^2$, and $E(e_i e_j) = 0$ for $i \neq j$, then the normalized, summed mean square error (J = SMSE) of $\hat{y}$ may be expressed as the sum of a bias term and a variance term. J = Bias Term + Variance Term = B + V, where

$$B = \frac{n}{m\sigma^2} \Sigma_{i=1}^{m} \{E[\hat{y}(\underline{x}_i)] - \eta(\underline{x}_i)\}^2 ,$$

and

$$V = \frac{n}{m\sigma^2} \Sigma_{i=1}^{m} \mathrm{Var}[\hat{y}(\underline{x}_i)] .$$

The KMH approach is used to achieve acceptably small levels of J. First an estimator $\underline{b}_1$ is selected so as to minimize the bias term B, and then an experimental design R^* with acceptably small variance term V is chosen to satisfy other design criteria desired by the experimenter.

Since the second derivative of the bias term B with respect to $E(\underline{b}_1)$ involves a positive definite matrix, minimum B is achieved by setting the first derivative equal to zero to get:

$$E(\underline{b}_1) = \underline{\beta}_1 + H_{11}^{-1}H_{12}\underline{\beta}_2 = [I \vdots H_{11}^{-1}H_{12}]\underline{\beta} = G\underline{\beta} .$$

In the finite region R, the regional moments are equal to $H_{ij} = m^{-1}X_i'X_j$. The expected value of $\underline{b}_1$ is:

$$E(\underline{b}_1) = E(T'\underline{y}^*) = T'\underline{\eta}^* = T'[X_1^* \vdots X_2^*]\underline{\beta} = T'X^*\underline{\beta} .$$

Therefore, the matrix T is the solution to the matrix equation $T'X^* = G$.

If the generalized inverse of a matrix S is denoted by S^-, then a necessary and sufficient condition for the solution of the matrix equation is $G(X'^*X^*)^-X'^*X^* = G$ (i.e., $G\underline{\beta}$ must be estimable). When this necessary and sufficient condition is satisfied, the minimum bias estimator which gives smallest variance for a fixed design is:

$$\underline{b}_{MB} = G(X'^*X^*)^-X'^*\underline{y}^* .$$

Substituting the MBE into the bias term, the minimum value of B is:

$$B_{MB} = \frac{n}{\sigma^2}\underline{\beta}_2'(H_{22} - H_{12}'H_{11}^{-1}H_{12})\underline{\beta}_2 .$$

The value of B_{MB} is the same for every design in the class of designs that allow the existence of the MBE.

If the OLS estimator $\underline{b}_{LS} = (X_1'^*X_1^*)^{-1}X_1'^*\underline{y}^*$, is used instead of the MBE, the value of the bias term B is:

$$B_{LS} = \frac{n}{\sigma^2}\underline{\beta}_2'(M_{12}'M_{11}^{-1}H_{11}M_{11}^{-1}M_{12} - 2M_{12}'M_{11}^{-1}H_{12} + H_{22})\underline{\beta}_2 .$$

B_{LS} does not have a constant value over all designs and is at least as large as B_{MB} (i.e., $B_{MB} \leq B_{LS}$).

When designs satisfy the BD condition, they also satisfy the KMH estimability condition because $E(\underline{b}_{LS}) = [I \vdots M_{11}^{-1}M_{12}]\underline{\beta} = [I \vdots H_{11}^{-1}H_{12}]\underline{\beta}$. Therefore, those designs that satisfy the BD condition are a subclass of all designs that satisfy the minimum bias condition. For this subclass of designs, the MBE becomes the OLS estimator. In general, the MBE is the sum of the OLS estimator and another component which is the product of the matrices contained in the BD condition and a $k \times 1$ vector, i.e.,

$$\underline{b}_{MB} = \underline{b}_{LS} + (H_{11}^{-1}H_{12} - M_{11}^{-1}M_{12})D^{-}X_2'^{*}F\underline{y}^{*}$$

where

$$F = [I - X_1^{*}(X_1'^{*}X_1^{*})^{-1}X_1'^{*}] \quad \text{and} \quad D = X_2'^{*}FX_2^{*} .$$

Let $R' = (H_{11}^{-1}H_{12} - M_{11}^{-1}M_{12})D^{-}X_2'^{*}$. Then the variance term for the MBE can be expressed as the sum to two traces:

$$V_{MB} = n\,\mathrm{Tr}[H_{11}(X_1'^{*}X_1^{*})^{-1}] + n\,\mathrm{TR}[H_{11}R'R] .$$

The first trace is the variance term of the OLS estimator and the second trace is of a non-negative definite matrix. Since both trace terms are non-negative, $V_{MB} \geq V_{LS}$. Equality holds if and only if the MBE becomes the OLS estimator.

When an experimenter is using designs that satisfy the BD condition, both the BD and KMH method give the OLS estimator and therefore, the same variance term V and bias term B. However, using the KMH method, the experimenter has the advantage of choosing from a larger class of designs while still minimizing the bias term B, and thus obtain greater design flexibility to meet other criteria which an experimenter may wish to impose on the design. The KMH method is illustrated when the true experimental model for a 2^r factorial design which consists of the mean, the main effects, and the two-factor interactions is approximated by a function containing only the estimated mean and the estimated main effects.

3. 2^r FACTORIAL EXPERIMENTS

To illustrate the notation to be used in a general 2^r factorial experiment, consider an example with $r = 2$ factors. For a 2^2 factorial design the true model before reparameterization is $\underline{\eta} = Z_1\underline{c}_1 + Z_2\underline{c}_2$ or:

$$\begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \\ \eta_4 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} \mu \\ T_{11} \\ T_{12} \\ T_{21} \\ T_{22} \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} (T_{12})_{11} \\ (T_{12})_{12} \\ (T_{12})_{21} \\ (T_{12})_{22} \end{bmatrix},$$

where in a 2^r factorial design, μ denotes the overall mean; T_{ig} the i^{th} factor, ($i = 1, 2, \ldots, r$) at the g^{th} level, $g = 1, 2$; and $(T_{ij})_{gh}$ the two-factor interaction of the i^{th} and j^{th} factors at the g^{th} and h^{th} level. The column vector $(\underline{z}_{ij})_{gh}$ associated with the $(T_{ij})_{gh}$ parameter is derived by multiplying the corresponding elements of the main effect column vectors $\underline{z}_{ig}$ and $\underline{z}_{jh}$. This elementwise multiplication of vectors is called a Hadamard product [10] and will be denoted by $\underline{z}_{ig} \odot \underline{z}_{jh} = (\underline{z}_{ij})_{gh}$. Using the Hadamard product, the true response for the 2^2 factorial example may be written as a linear combination of the vector $\underline{z}_0 = \underline{1}$ (i.e., a vector of ones) and the vectors associated with the main effects;

$$\underline{\eta} = \mu\underline{z}_0 + \Sigma_{i=1}^{2} \Sigma_{g=1}^{2} T_{ig}\underline{z}_{ig} + \Sigma_{g=1}^{2} \Sigma_{h=1}^{2} (T_{12})_{gh}(\underline{z}_{1g} \odot \underline{z}_{2h}) .$$

In the true model, the Z_1 matrix is reparameterized to the matrix X_1 of full column rank. For a 2^r factorial experiment, the orthogonal reparameterization of $\underline{x}_i = \underline{z}_{i1} - \underline{z}_{i2}$, $i = 1, \ldots, r$; is used, so that for each factor, the high level is denoted by a plus one (+1) and the low level is denoted by a minus one (-1). The set of all 2^r reparameterized column vectors for a complete factorial experiment is denoted by the set $FD(2^r) = \{\underline{x}_0; \underline{x}_1, \ldots, \underline{x}_r; \underline{x}_1 \odot \underline{x}_2, \underline{x}_1 \odot \underline{x}_3, \ldots; \ldots; \ldots; \underline{x}_1 \odot \ldots \odot \underline{x}_r\}$. These column vectors are linearly independent and orthogonal. The mean column vector is a vector of ones (i.e., $\underline{x}_0 = \underline{1}$), and the interaction column vectors are the Hadamard products of main effect column vectors. The group of column vectors in the matrix X_1 is a subset of the FD(2^r) column vectors consisting of the mean column vector and the main effect column vectors, i.e., $X_1 = (\underline{x}_0, \underline{x}_1, \ldots, \underline{x}_r)$.

Let the parameter $F_i = T_{i1} - T_{i2}$ represent the i^{th} factor. Then the reparameterized true model; $\underline{\eta} = X_1\underline{\beta}_1 + X_2\underline{\beta}_2$ for the 2^2 factorial example is:

$$\begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \\ \eta_4 \end{bmatrix} = \begin{bmatrix} 1 & +1 & +1 \\ 1 & +1 & -1 \\ 1 & -1 & +1 \\ 1 & -1 & -1 \end{bmatrix} \begin{bmatrix} \mu \\ F_1 \\ F_2 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} (T_{12})_{11} \\ (T_{12})_{12} \\ (T_{12})_{21} \\ (T_{12})_{22} \end{bmatrix} .$$

For a general 2^r factorial experiment, the second order model may be written as a linear combination of the vectors $\underline{x}_0$, x_i, and $(\underline{z}_{ig} \odot \underline{z}_{jh})$, for $g = 1, 2$ and $h = 1, 2$:

$$\eta = \mu\underline{x}_0 + \Sigma_{i=1}^{r} F_i\underline{x}_i + \Sigma_{i=1}^{r-1} \Sigma_{j=i+1}^{r} \Sigma_{g=1}^{2} \Sigma_{h=1}^{2} (T_{ij})_{gh}(\underline{z}_{ig} \odot \underline{z}_{jh}). \qquad (3.1)$$

The parameters in the approximating function for the second order model in (3.1) are estimated from a fraction of the points in a complete 2^r factorial design. The construction of these fractional factorial designs is described in the next section.

3.1 Factional Factorial Designs

The second order model in (3.1) is approximated by a first order function, $\hat{\underline{y}} = X_1^*\underline{b}_1$ consisting of an estimated mean and estimated main effects:

$$\hat{\underline{y}} = \hat{\mu}\underline{x}_0^* + \Sigma_{i=1}^{r} \hat{F}_i\underline{x}_i^* . \qquad (3.2)$$

An $n \times 1$ column vector in the experimental design matrix $X_1^* = (\underline{x}_0^*, \underline{x}_1^*, \ldots, \underline{x}_r^*)$ is formed from a subset of elements in the corresponding column vector in the matrix $X_1 = (\underline{x}_0, \underline{x}_1, \ldots, \underline{x}_r)$. For each experimental design of n-points, there is a set of 2^r column vectors which is called a fractional factorial design FFD(n) $= \{\underline{x}_0^*, \underline{x}_1^*, \ldots, \underline{x}_r^*; \underline{x}_1^* \odot \underline{x}_2^*, \ldots; \ldots; \ldots; \underline{x}_1^* \odot \ldots \odot \underline{x}_r^*\}$ corresponding to the FD(2^r) set. Since the number of experimental points is $n \leq m$, the column vectors in FFD(n) are not linearly independent unless $n = m$. Fractional factorial designs are constructed by specifying linear relationships that the column vectors of FFD(n) must satisfy.

Two column vectors $\underline{x}^*$ and $\underline{y}^*$ in FFD(n) are said to be aliased if $\underline{x}^* = \underline{+} a\underline{y}^*$, for $a > 0$. The alias scalar, $\underline{+} a$, is taken to be $\underline{+} 1$ in 2^r factorial experiments. Fractional factorial designs in this paper are constructed by specifying the column vectors in FFD(n) that are aliased with the mean column vector (i.e., $\underline{x}_0^* = \underline{1}$). The column vectors form an identity relation set (IDR) and this set is denoted by setting "I" equal to the letters representing the factors or interaction of factors that are aliased with $\underline{x}_0^*$. For example, the IDR, I = + ABC = - CDE = - ABDE means the following column vectors in FFD(n) are aliased: $\underline{x}_1^* \odot \underline{x}_2^* \odot \underline{x}_3^* = \underline{x}_0^*$, $\underline{x}_3^* \odot \underline{x}_4^* \odot \underline{x}_5^* = - \underline{x}_0^*$, and $\underline{x}_1^* \odot \underline{x}_2^* \odot \underline{x}_4^* \odot \underline{x}_5^* = - \underline{x}_0^*$. Each column vector in an IDR is called a word and the Hadamard product of any two words forms a word that is also in the IDR. A subset of words (called generators) that are not the Hadamard products of each other, generate the remaining words by taking the Hadamard product of all possible combinations of these generators. From a set of s-generators, $2^s - s - 1$ words can be generated to give a total of $2^s - 1$ words in the IDR. Therefore, only the generators need be specified to define an IDR. Two IDR's with the same generators, but with different alias scalars are said to belong to the same IDR family.

If the number of points in a $K(2^{r-s})$ fraction of a 2^r factorial design is $n = 2^{r-s}$ (i.e., K = 1), then the design is called a regular fraction. Regular fractions can be combined to form fractional factorial designs with $n = K(2^{r-s})$ points (K = 3, 5, ...) which are called irregular fractions. The column vectors for the main effects of an irregular fraction with $K(2^{r-s})$ points are constructed by combining the main effect column vectors of K regular fractions from the same IDR family.

Regular and irregular fractions are classified by the order of the effects that can be estimated from the design. If main effects are called first order effects, two-factor interactions are called second order effects, etc., and those effects that are assumed to be zero or near zero are called negligible, then a fractional factorial design is of even or odd resolution [7] if:

Resolution	Order of Estimable Effects	Order of Negligible Effects
2t + 1	t or less	t + 1 or greater
2t	t - 1 or less	t + 1 or greater

for regular fractions, the resolution of the fraction is equal to the length of the smallest word in the IDR.

3.2 Approximating A Second Order Model With A First Order Function

The regional moments for the second order model in a 2^r factorial are $H_{11} = m^{-1}X_1'X_1 = m^{-1}mI_p = I_p$ the identity matrix of size $p = r + 1$, and the matrix $H_{12} = m^{-1}(\underline{x}_0, \underline{x}_1, \ldots, \underline{x}_r)' (\underline{z}_{11} \odot \underline{z}_{21}, \ldots, \underline{z}_{r-1,2} \odot \underline{z}_{r2})$. Since the interaction column vectors $(\underline{z}_{ig} \odot \underline{z}_{jh})$ are related to the column vectors in $FD(2^r)$ by:

$$(\underline{z}_{ig} \odot \underline{z}_{jh}) = (-1)^{g+h}[\underline{x}_i \odot \underline{x}_j + (-1)^{h+1}\underline{x}_i + (-1)^{g+1}\underline{x}_j + (-1)^{g+h}\underline{1}]/4 ,$$

each element in the matrix H_{12} can be found using the properties of Hadamard products. Therefore, if the estimator $\underline{b}_1$ in the first order approximating function (3.2) is to be a MBE, a design X_1^* must be chosen so that $E(\underline{b}_1) = G\underline{\beta} = [I \vdots H_{11}^{-1}H_{12}]\underline{\beta}$ is estimable, or

$$E(\hat{\mu}) = \mu + 1/4 \Sigma_{i=1}^{r-1} \Sigma_{j=i+1}^{r} \Sigma_{g=1}^{2} \Sigma_{h=1}^{2} (T_{ij})_{gh}$$

$$E(\hat{F}_\rho) = F_\rho + 1/4 \Sigma_{i=1}^{\rho-1} \Sigma_{g=1}^{2} \Sigma_{h=1}^{2} (-1)^{h+1}(T_{i\rho})_{gh}$$

$$+ 1/4 \Sigma_{j=\rho+1}^{r} \Sigma_{g=1}^{2} \Sigma_{h=1}^{2} (-1)^{g+1}(T_{\rho j})_{gh} \quad \text{for} \quad \rho = 1, 2, \ldots, r .$$

If an experimental design allows a MBE, there must exist vectors $\underline{a}$ and $\underline{b}_\rho$, $\rho = 1, 2, \ldots, r$; so that the expected values of the vector of observed responses $\underline{y}^*$, from the experimental design are: $E(\underline{a}'\underline{y}^*) = E(\hat{\Omega})$ and $E(\underline{b}_\rho'\underline{y}^*) = E(\hat{F}_\rho)$ for every ρ. However, $E(\underline{a}'\underline{y}^*) = \underline{a}'\underline{\eta}^*$ and $E(\underline{b}_\rho'\underline{y}^*) = \underline{b}_\rho'\underline{\eta}^*$ for every ρ. By equating expected values, the following identities for the vectors $\underline{a}$ and $\underline{b}_\rho$, $\rho = 1, 2, \ldots, r$ can be derived; $\underline{a}'\underline{x}_0^* = 1$, $\underline{a}'\underline{x}_i^* = 0$, $i = 1, 2, \ldots, r$; $\underline{a}'(\underline{x}_i^* \odot \underline{x}_j^*) = 0$ for every i and j; and $\underline{b}_\rho'\underline{x}_0^* = 0$, $\underline{b}_\rho'\underline{x}_\rho^* = 1$, $\underline{b}_\rho'\underline{x}_q^* = 0$ for $q = 1, 2, \ldots, r$, $q \neq \rho$; $\underline{b}_\rho'(\underline{x}_i^* \odot \underline{x}_j^*) = 0$ for every i and j. These identities lead to the condition that there are no linear dependencies involving main effect column vectors in the subset of column vectors for the mean, main effects and two-factor interactions from the FFD(n) set. This condition is a necessary and sufficient condition for a fractional factorial design to be resolution IV [9].

THEOREM 3.1

If a fractional factorial design allows the existence of a MBE, then the design must be a resolution IV design with at least 2r design points.

An example of a fractional factorial design that allows the existence of a MBE and has a minimum number of points is a 2^{4-1} design that is defined by the IDR, I = + ABCD. The converse of Theorem 3.1 is not true in general, but for regular fractions the converse is true.

THEOREM 3.2

If a regular fraction is a resolution IV design, then the design allows the existence of a MBE.

Proof:

To prove this theorem the assumptions are shown to imply that the BD condition holds.

Because regular fractions of resolution IV or higher satisfy the BD condition, the MBE becomes the OLS estimator. Therefore, the minimum bias term B is minimized by using regular fractions that are resolution IV designs.

If K-regular fractions are combined, an irregular fraction with $n = K(2^{r-s})$ points can be constructed. For example, a $3(2^{4-2})$ irregular fraction can be constructed by combining three regular 2^{4-2} designs that are defined by the same IDR family; I = ± AD = ± BCD = ± ABC. If the IDR for each regular fraction is:

Fraction 1: I = + AD = + BCD = + ABC ,

Fraction 2: I = - AD = - BCD = + ABC ,

Fraction 3: I = - AD = + BCD = - ABC ,

then the $3(2^{4-2})$ irregular fraction is represented by the following:

IDR	Fraction 1	2	3
AD	+	-	-
BCD	+	-	+
ABC	+	+	-

For this example, four different sets of three IDR's could have been chosen to construct the irregular fraction. In general, which of the $\binom{2^s}{K}$ possible regular fractions from the same IDR famile are used to construct an irregular fraction does not affect the existence or non-existence of a MDK, the value of the variance term V, or the value of the bias term R.

However, in order to have a consistent method of constructing irregular fractions, Addelman's method [1] is used to choose the different regular fractions from an IDR family. For the irregular fractions that are studied in this paper K is an odd number, so Addelman's method assigns an odd number of the K alias scalars equal to -1 for IDR words of odd length and an even number of the K alias scalars equal to -1 for IDR words of even lengths.

An important class of irregular fractions are those which are constructed by combining resolution IV, regular fractions.

THEOREM 3.3

If an irregular fraction is constructed by combining regular fractions of resolution IV, then the design allows the existence of a MBE.

Proof:

As in Theorem 3.2, the assumptions are shown to imply that the BD condition holds.

For seven or more factors there always exist resolution IV, 2^{r-2} and 2^{r-3} regular fractions. Therefore, Theorem 3.3 guarantees that we can always combine these regular fractions to form $K(2^{r-2})$ and $K(2^{r-3})$ irregular fractions which allow MBE. Regular fractions which have resolution less than IV may also be combined to form irregular fractions that allow MBE. To demonstrate this fact, the estimability of $G\underline{\beta}$ was examined by using a computer program for $3(2^{r-2})$ and $3(2^{r-2})$ irregular fractions constructed from regular fractions of resolution IV or less for r = 3, 4, 5 and 6.

The generators of the defining IDR family were selected systematically according to their word length and by how many letters each generator has in common with the other generators. For the $3(2^{r-2})$ irregular fractions, there are no designs that allow a MBE if r = 3, and no $3(2^{r-3})$ irregular fractions exist that allow a MBE for $r \leq 5$. Those irregular fractions which allow the existence of a MBE are listed in Table 1 for $3(2^{6-3})$ designs and in Table 2 for $3(2^{r-2})$ designs for r = 4, 5 and 6. Each design in Tables 1 and 2 is classified by an N-tuple ($N = 2^s - 1$) of the lengths of the words in the defining IDR family. For each design that allows the existence of a MBE, the values of the variance term V for the MBE and the OLS estimator are listed in the tables. If the values of the two variance terms are equal, then the MBE and the OLS estimator are equivalent. The only design in the two tables where the values of the variance terms are equal is for the $3(2^{6-2})$ design (4,4,4). For this design, each word length in the defining IDR family is four, so by Theorem 3.3, this design also satisfies the BD condition.

The advantage of using the MBE rather than the OLS estimator is illustrated for the irregular $3(2^{6-2})$ fraction (2,4,6). Let J_{LS} = SMSE for the OLS estimator, J_{MB} = SMSE for the MBE, $\underset{\sim}{ab}$ = the vector of parameters $(ab_{11}, ab_{12}, ab_{21}, ab_{22})'$, and

$$A = \begin{bmatrix} +1 & -1 & -1 & +1 \\ -1 & +1 & +1 & -1 \\ -1 & +1 & +1 & -1 \\ +1 & -1 & -1 & +1 \end{bmatrix} .$$

Then the increase obtained in the SMSE using the OLS estimator rather than the MBE is:

$$J_{LS} - J_{MB} = (3/\sigma^2)\underset{\sim}{ab}'A\underset{\sim}{ab} - 0.375 .$$

By graphing $J_{LS} - J_{MB}$ versus the non-negative quadratic form $\underset{\sim}{ab}'A\underset{\sim}{ab}/\sigma^2$ (Figure A), one can see that the OLS estimator should be used only if $\underset{\sim}{ab}'A\underset{\sim}{ab}$ has a value less than 1/8 the sampling variance σ^2. The size of $\underset{\sim}{ab}'A\underset{\sim}{ab}$ is a measure of the non-negligibility of the two-factor interactions. Even if the MBE is used in this situation, the maximum increase in J_{MB} over J_{LS} is only 0.375, which is approximately 5% of the variance term V_{LS}. However, if the OLS estimator is always used, the increase in J_{LS} over J_{MB} can be quite large and in fact is not bounded.

3.3 Example

All of the designs that allow a MBE in Section 3 are for a full second order model (3.1) being approximated by a first order function (3.2). If additional knowledge is available about some of the two-factor interaction terms so they can be eliminated from the true model (3.2), then designs that allow MBE may exist where they did not exist using the full second order model. For example, suppose an experiment is conducted using three chemicals (i.e., a, b, and c) each at two concentrations and it is known that the chemical "c" can not react with chemicals "a" and "b". The true model is assumed to be $\eta_{ijk} = \mu + a_i + b_j + c_k + (ab)_{ij}$ for i, j and k = 1, 2, but the chemist wants to use the simpler approximating function $\hat{y}_{ijk} = \hat{\mu} + \hat{a}_i + \hat{b}_j + \hat{c}_k$ basing the estimators on a six point design. For the full second order model there are no $3(2^{3-2})$ designs that allow a MBE, but by eliminating two of the two-factor interactions a MBE does exist for each of the following irregular fractions:

Design (1,1,2)

IDR	Fraction 1 2 3
A	+ + -
C	+ - +
AC	+ - -

Design (1,2,3)

IDR	Fraction 1 2 3
A	+ - +
BC	+ - -
ABC	+ + -

Design (2,2,2)

IDR	Fraction 1 2 3
AB	+ - -
BC	- + -
AC	- - +

The SMSE for these three designs are listed in Table 3.

The individual values of J are plotted for each of the three designs in Figure B versus the non-negative quadratic form $\underline{ab}'A\underline{ab}/\sigma^2$. Adopting the SMSE criterion to choose the "best" of the three designs, for minimum bias estimation, only the variance term V (i.e., intercept) of the J_{MB}'s need be considered since all three designs yield the same bias term B (i.e., the J_{MB} lines have identical slopes). Because the smallest variance term V for the J_{MB}'s is 5.250 for the design (1,2,3) it is the optimal choice which is contrary to the situation resulting when OLS estimation is used. The SMSE J_{LS} for design (1,2,3) has a smaller variance term V than the J_{LS} for the designs (1,1,2) and (2,2,2), as is also true for the MBE. However, the bias term B (i.e., the slope) for design (1,2,3) is larger than the bias term B for designs (1,1,2) and (2,2,2). In the presence of a non-negligible AB interaction, the larger bias term (1.35 times as large) would make the design (1,2,3) less appealing than either of the other two designs when OLS estimation is used.

4. SUMMARY AND CONCLUSIONS

The KMH method of minimum bias estimation has been applied to the classical experimental design model with factors having a finite number of levels. For this situation, the MBE gives the minimum bias term B for the SMSE which, in general, is smaller than the bias term B using the OLS estimator. The variance term V for the MBE is greater or equal to the variance term V for the OLS estimator, and equality occurs if and only if the two estimators are equal. The MBE does become the OLS estimator on the subclass of designs satisfying the Box-Draper condition which are contained in the class of all designs allowing the existence of a minimum bias estimator.

For 2^r factorial experiments, factional factorial designs were investigated when a second order model was approximated by a first order function. A sufficient condition for designs to allow the existence of a MBE is that the fractional factorial design must be of resolution IV. For regular fractions, resolution IV is also a necessary condition for the design to satisfy the Box-Draper condition and therefore, allow a MBE. Irregular fractions that are constructed by combining resolution IV, regular fractions also satisfy the Box-Draper condition. However, examples of irregular fractions constructed from regular fractions of resolution less than IV which allow the existence of a MBE are given for $3(2^{6-3})$ irregular fractions in Table 1 and $3(2^{r-2})$ irregular fractions in Table 2 for $r = 4$, 5, and 6.

TABLE 1 $3(2^{6-3})$ irregular fractions

Factor	No. of Design Points	Design	Min. Bias	Generators Of The IDR Family	Min. Bias Variance Term	Least Sq. Variance Term
6	24	(1,1,1,2,2,2,3)	No	A,B,C		
	24	(1,1,2,2,3,3,4)	No	A,B,CD		
	24	(1,1,2,3,4,4,5)	No	A,B,CDE		
	24	(1,1,2,4,5,5,6)	No	A,B,CDEF		
	24	(1,2,2,2,3,3,3)	No	A,BC,CD		
	24	(1,2,2,3,3,4,5)	No	A,BC,DE		
	24	(1,2,3,3,3,4,4)	No	A,BC,CDE		
	24	(1,2,3,3,4,5,6)	No	A,BC,DEF		
	24	(1,2,3,4,4,5,5)	No	A,BC,CDEF		
	24	(1,3,3,4,4,4,5)	No	A,BCD,DEF		
	24	(2,2,2,2,2,2,4)	No	AB,BC,CD		
	24	(2,2,2,2,4,4,4)	No	AB,BC,DE		
	24	(2,2,2,3,3,4,4)	No	AB,BC,CDE		
	24	(2,2,2,3,5,5,5)	No	AB,BC,DEF		
	24	(2,2,2,4,4,4,6)	No	AB,BC,CDEF		
	24	(2,2,2,4,4,4,6)	No	AB,CD,EF		
	24	(2,2,3,3,3,3,4)	No	AB,CD,ACE		
	24	(2,2,3,3,4,5,5)	Yes	AB,CD,AEF	9.750	7.500
	24	(2,2,4,4,4,4,4)	Yes	AB,CD,ACEF	8.000	7.500
	24	(2,3,3,3,3,4,6)	Yes	AB,BCD,AEF	10.125	7.250
	24	(2,3,3,3,4,4,5)	Yes	AB,CDE,ACF	9.375	7.250
	24	(3,3,3,3,4,4,4)	No	ABC,CDE,ADF		

TABLE 2 $3(2^{r-2})$ irregular fractions for r = 4, 5, and 6

Factor	No. Of Design Points	Design	Min. Bias	Generators Of The IDR Family	Min. Bias Variance Term	Least Sq. Variance Term
4	12	(1,1,2)	No	A, B		
	12	(1,2,3)	No	A, BC		
	12	(1,3,4)	Yes	A, BCD	6.750	5.250
	12	(2,2,2)	No	AB, BC		
	12	(2,2,4)	Yes	AB, CD	6.000	5.500
	12	(2,3,3)	Yes	AB,BCD	7.125	5.250
5	24	(1,1,2)	No	A, B		
	24	(1,2,3)	No	A, BC		
	24	(1,3,4)	Yes	A, BCD	7.875	6.250
	24	(1,4,5)	Yes	A, BCDE	6.750	6.250
	24	(2,2,2)	No	AB, BC		
	24	(2,2,4)	Yes	AB, CD	7.000	6.500
	24	(2,3,3)	Yes	AB, BCD	8.125	6.250
	24	(2,3,5)	Yes	AB, CDE	6.750	6.250
	24	(2,4,4)	Yes	AB, BCDE	6.375	6.250
	24	(3,3,4)	Yes	ABC, CDE	7.000	6.000
6	48	(1,1,2)	No	A, B		
	48	(1,2,3)	No	A, BC		
	48	(1,3,4)	Yes	A, BCD	9.000	7.250
	48	(1,4,5)	Yes	A, BCDE	7.875	7.250
	48	(1,5,6)	Yes	A, BCDEF	7.875	7.250
	48	(2,2,2)	No	AB, BC		
	48	(2,2 4)	Yes	AB, CD	8.000	7.500
	48	(2,3,3)	Yes	AB, BCD	9.125	7.250
	48	(2,3,5)	Yes	AB, CDE	7.750	7.250
	48	(2,4,4)	Yes	AB, BCDE	7.750	7.250
	48	(2,4,6)	Yes	AB, CDEF	7.375	7.250
	48	(2,5,5)	Yes	AB, BCDEF	7.375	7.250
	48	(3,3,4)	Yes	ABC, CDE	8.000	7.000
	48	(3,3,6)	Yes	ABC, DEF	7.750	7.000
	48	(3,4,5)	Yes	ABC, CDEF	7.375	7.000
	48	(4,4,4)	Yes	ABCD, CDEF	7.000	7.000

TABLE 3 The SMSE of $3(2^{3-2})$ designs for the true model: $\eta_{ijk} = \mu + a_i + b_j + c_k + (ab)_{ij}$

Design	Estimator	SMSE
(1,2,3)	Least Squares	$J_{LS} = (9/2\sigma^2)\underline{ab}'A\underline{ab} + 4.500$
	Minimum Bias	$J_{MB} = (3/\sigma^2)\ \underline{ab}'A\underline{ab} + 5.250$
(1,1,2)	Least Squares	$J_{LS} = (10/3\sigma^2)\underline{ab}'A\underline{ab} + 5.500$
	Minimum Bias	$J_{MB} = (3/\sigma^2)\ \underline{ab}'A\underline{ab} + 5.625$
(2,2,2)	Least Squares	$J_{LS} = (10/3\sigma^2)\underline{ab}'A\underline{ab} + 5.500$
	Minimum Bias	$J_{MB} = (3/\sigma^2)\ \underline{ab}'A\underline{ab} + 5.625$

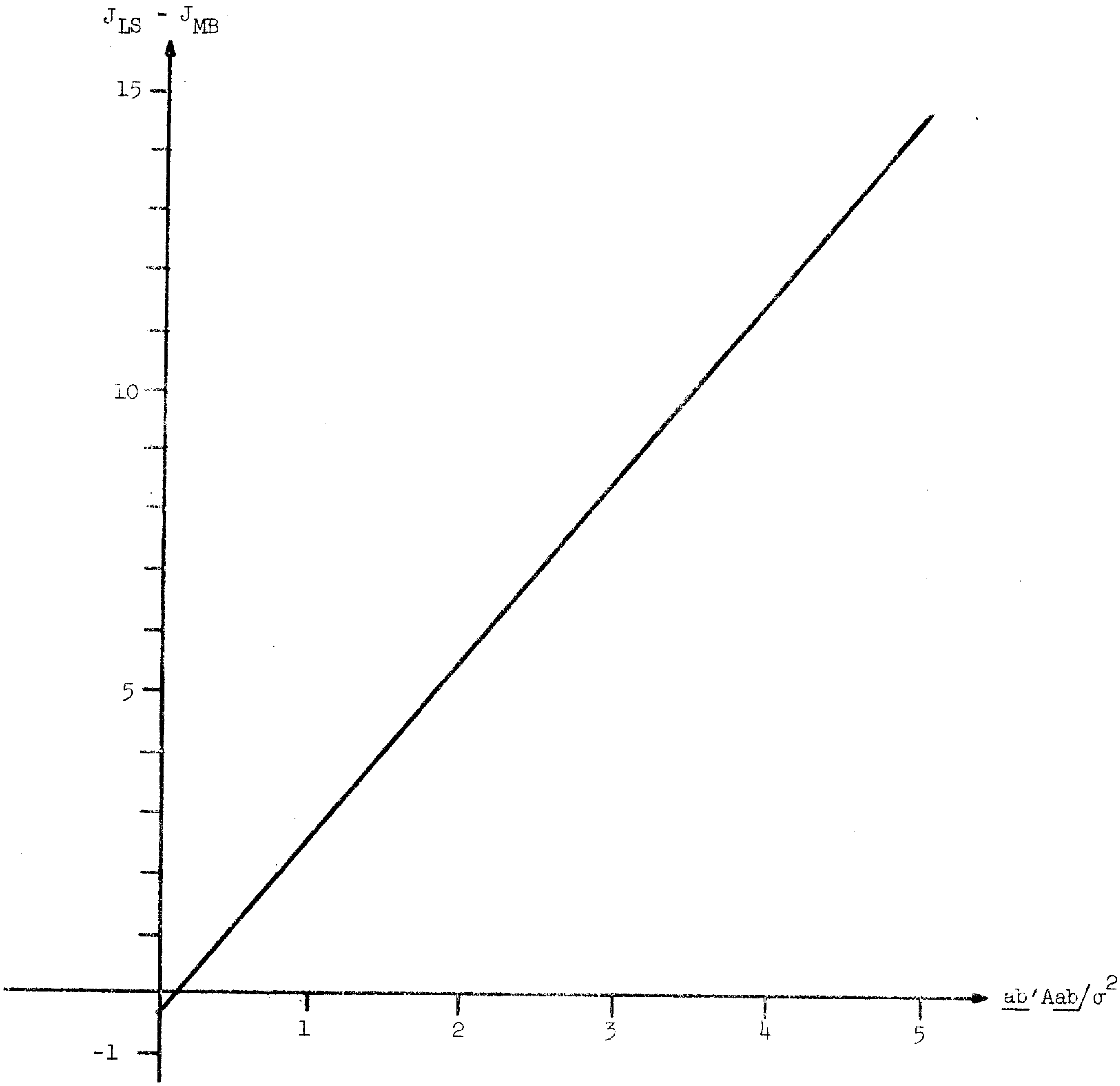

Figure A $J_{LS} - J_{MB}$ for the $3(2^{6-2})$ design (2,4,6)

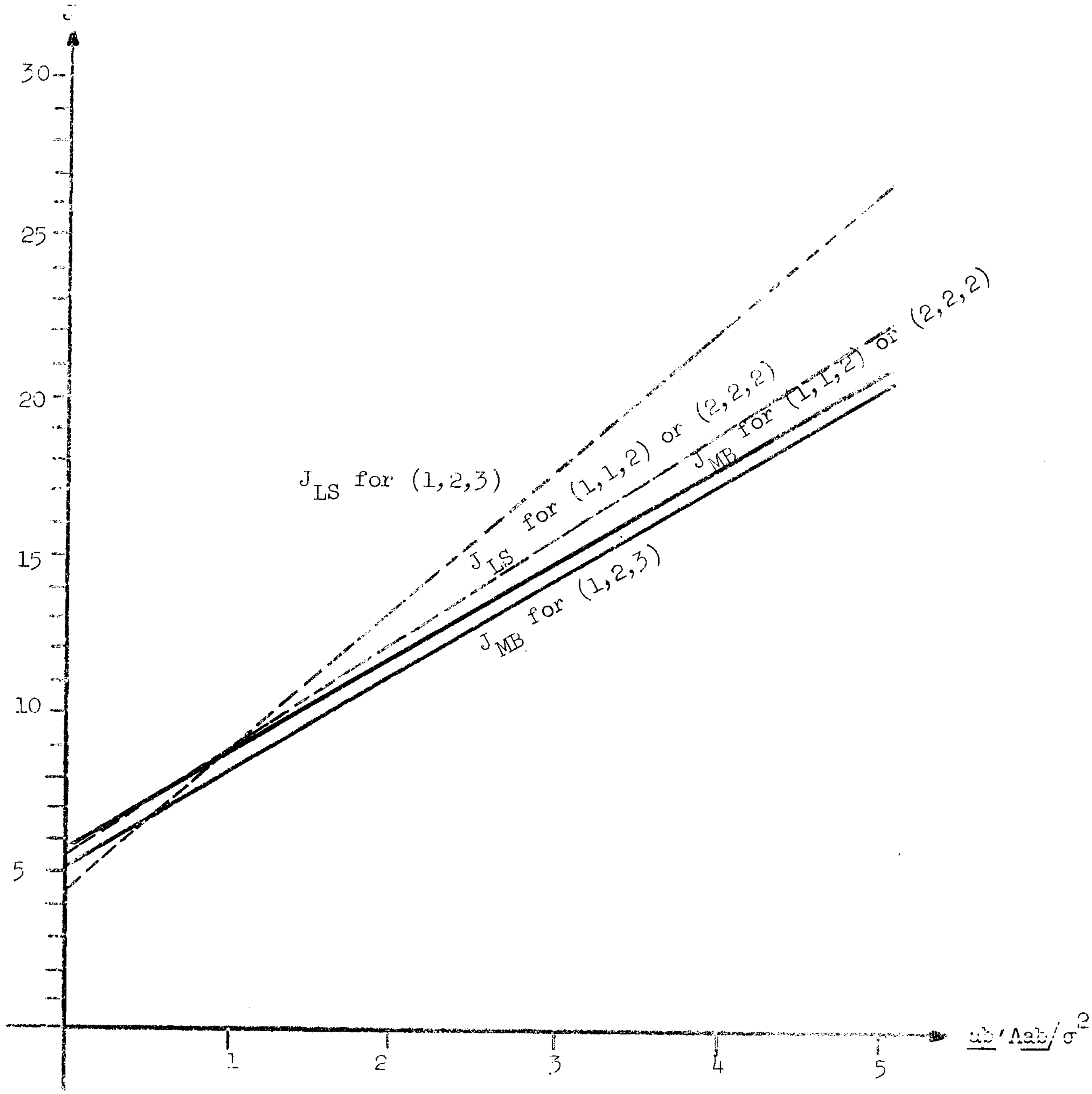

Figure B The SMSE's of $3(2^{3-2})$ designs for the true model:

$$\eta_{ijk} = \mu + a_i + b_j + c_k + (ab)_{ij}$$

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