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A NOTE ON CONSTRUCTING 2^n3^1 AND 2^13^3 DESIGNS WHEN LINEAR TERMS ARE ESSENTIAL

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ABSTRACT

Under the assumption that the three-level factors are quantitative, the linear effects are taken more attention than the quadratic effects of the interaction terms. Webb (1971) presented some small incomplete factorial designs that are mixed two- and three-level designs with 20 or fewer runs. The designs provided the estimating linear-by-linear components of interactions between the three-level factors; moreover, they could also offer estimation of interactions that interest the experiments. Webb used ad hoc methods to find these plans; hence, there was still no unified structure to those experiments. In this paper, we develop the methods to construct the 2^n3^1 and 2^13^3 designs. The designs constructed by these methods not only supply orthogonal estimates of all the main effects but also permit estimation of all the two-factor interactions not involving the quadratic effects. Furthermore, the designs we find are nearly orthogonal.

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1. INTRODUCTION

The constructions of the 2^n3^m designs are more complicated than the usual 2^n and 3^m designs. The mixed 2^n3^m series have been discussed by authors, such as Connor and Young (1961), Margolin (1969), Webb (1971), Wang and Wu (1992), and Wu and Hamada (2000). In Connor and Young's paper, they presented 39 pairs (m, n) that included from $m + n = 5$ through $m + n = 10$, $(m, n \neq 0)$. These plans permit estimation of all the main effects and two-factor interactions, but the main effects are not orthogonal to each other in some of their designs.

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Margolin used three techniques to obtain orthogonal main-effect designs with resolution V.

Webb concentrated other status and used ad hoc methods to construct small fractional factorial designs. He considered that the three-level factors were quantitative and assumed that the experimenters are more interested in the linear effects than in the quadratic effects of these factors. Hence, the only interactions that three-level factors and two-level factors considered by the experimenters are the terms involved linear effects. Unfortunately, most of the designs constructed by Webb are not the orthogonal main-effect plans; that is, the estimations of main effects are correlated with estimates of other main effects. In this paper, we are going to construct nearly orthogonal plans for 2^n3^1 and 2^13^3 designs.

This article is organized as follows. We give a brief description of the index first in section 2. We also develop a theorem and give an example to explain the idea of the 2^n3^1 designs. In section 3, we explore the properties of 2^13^3 designs. Conclusion is given in section 4.

2. THE 2^n3^1 DESIGNS

Occasionally an experimenter may need to decide the experimental runs according to some criteria. Although there are several optimal criteria in the literature, the design can not simultaneously satisfy the optimal conditions. Certain designs may only be available for some particular requirements. In order to obtain the overall information about the response at each treatment combination of factorial design, Webb (1971) used a criterion called the "fitting index" to select the design. By the property of index, a larger value of index is derivable for the design. The index is defined as follows:

$$I_F = \frac{p}{N\sum_{i=1}^{p} w_i K_i}$$

where p is the number of parameters in the model, N is the number of runs in the design, the K_i are the diagonal elements of the variance-covariance matrix $(\mathbf{X}^\mathbf{T}\mathbf{X})^{-1}$, and where the values of the w_i, related to the lengths of the column vectors of $\mathbf{X}$, are: grand mean "1", effect of two-level factor "1", linear effect of three-level factor "2/3", quadratic effect of three-level factor "2", interaction between two-level factors "1", interaction between a two- and a three-level factor "2/3", interaction between three-level factors "4/9". In general, an incomplete factorial performs more poorly than the full factorial by the criterion of index.

For the regular fractional factorial designs, the index is 100%, which makes these designs very attractive when they are available.

Let U be a three-level factor whose levels denote U_i, i=0, 1, and 2.

THEOREM 2.1. *Let M_1 and M_2 be two orthogonal main-effect plans with runs 2^{n-p} and 2^{n-r}, respectively. If $M_1 + M_2$ is a resolution V plan, then $M_1U_0 + M_2U_1 + M_1U_2$ is an orthogonal main-effect plan with $2^{n-p+1} + 2^{n-r}$ runs. In this design all the main effects and two-factor interactions not involving the quadratic effect could be estimated.*

PROOF. The contrast coefficients for the three-level factor are calculated as:
$\overline{X} = (0 \times 2^{n-p} + 1 \times 2^{n-r} + 2 \times 2^{n-p})/(2^{n-p+1} + 2^{n-r}) = 1$
so the linear coefficients are given by $0 - 1 = -1$, $1 - 1 = 0$, $2 - 1 = 1$.
And let $k = ((-1)^2 \times 2^{n-p} + 0^2 \times 2^{n-r} + 1^2 \times 2^{n-p})/(2^{n-p+1} + 2^{n-r})$,
then the quadratic coefficients are given by

$$(2^{n-p+1} + 2^{n-r})(1 - k) = 2^{n-r}, \qquad (2^{n-p+1} + 2^{n-r})(0 - k) = -2^{n-p+1},$$
$$(2^{n-p+1} + 2^{n-r})(1 - k) = 2^{n-r}.$$

That is, the linear and quadratic coefficients of three-level factor are -1, 0, 1 and 2^{n-r}, -2^{n-p+1}, 2^{n-r}, respectively. Let W_1 be the design matrix including the mean, two-level factors, and interactions between two-level factors. Let W_2 be the design matrix including not only linear and quadratic effects of the three-level factor but also interactions between two- and three-level (linear component) factors. Then the matrix would be formed

$$(\mathbf{X}^T\mathbf{X}) = (W_1 \;\; W_2)^T(W_1 \;\; W_2) = \begin{bmatrix} W_1^TW_1 & W_1^TW_2 \\ W_2^TW_1 & W_2^TW_2 \end{bmatrix}$$

Let T_i be a two-level factor ($i = 1, 2, .., n$). Since M_1 and M_2 are orthogonal main-effect plans, Sum(X_{T_i})=Sum(X_{TiTj}) $= 0$ on both plans. Hence, we have the same result in $M_1U_0+M_2U_1+M_1U_2$ plan. On the other hand, we will observe Sum(X_{TiUl}) = Sum(X_{TiUq}) = Sum(X_{TiTjUl}) = Sum(X_{TiTjUq}) = Sum(X_{Ti^2TjUl}) = Sum(X_{Ti^2Ul}) = 0 on $M_1U_0 + M_2U_1 + M_1U_2$, where the X_{Ti} is the orthogonal contrast defining the corresponding effect. And the notation "Sum", for convenience, express the sum of the column vector. The column vectors X_{TiTjTk} are the same in the first and third plan. The column vectors X_{Ul} have opposite sign on both plans, hence $\text{Sum}(X_{TiTjTkUl}) = 0$. These relations imply that $W_1^T W_2$ and $W_2^T W_1$ are zero matrices. Similarly, we could show that $W_2^T W_2$ is a diagonal matrix. From the assumption, $M_1 + M_2$ is an orthogonal main-effect plan with resolution V, and then we have the conclusion that $W_1^T W_1$ is a nonsingular matrix and the theorem is proved. □

EXAMPLE 2.1. The $2^3 3^1$ design with 12 runs.
Suppose that M_1 and M_2 are two orthogonal main-effect plans with resolution III defined by $I = -ABC$, and $I = ABC$. Hence $M_1 + M_2$ is a resolution V design with 8 runs. Then $M_1U_0 + M_2U_1 + M_1U_2$ (see Table 2.1) is an orthogonal main effect plan that all two-factor interactions not involving quadratic term can be estimated according to theorem 2.1.

Webb also presented this kind of design, which is shown in Table 2.2. Webb claimed that the design provided the estimation of the following effects: A, B, C, Ul, Uq, AB, AC, AUl, BUl, and CUl. The index is 67% in this situation. In fact, we can estimate the effects A, B, C, Ul, Uq, AB, AC, BC, AUl, BUl, and CUl from the design. The regression model is fitted by

$$E(Y) = \beta_0 + \beta_1 X_A + \beta_2 X_B + \beta_3 X_C + \beta_{12} X_{AB} + \beta_{13} X_{AC} + \beta_{23} X_{BC}$$
$$+\beta_4 X_{Ul} + \beta_5 X_{Uq} + \beta_6 X_{AUl} + \beta_7 X_{BUl} + \beta_8 X_{CUl}$$

The diagonal entries of $(\mathbf{X}^\mathbf{T}\mathbf{X})^{-1}$ are: 0.164, 0.118, 0.118, 0.201, 0.118, 0.201, 0.201, 0.306, 0.062, 0.306, 0.306, and 0.472. Hence, the index is obtained by

$\sum_{i=1}^{12} w_i K_i = (0.164 + 0.118 \times 3 + 0.201 \times 3) + (2/3) \times (0.306 \times 3 + 0.472) + (2 \times 0.062) = 2.172$
$I_F = 12/(12 \times 2.172) = 46\%$

For the new design, the index is 96% if the model does not contain the BC effect. Suppose that the BC interaction is added to the model, then the diagonal elements of $(\mathbf{X}^\mathbf{T}\mathbf{X})^{-1}$ are: 0.083, 0.094, 0.094, 0.094, 0.094, 0.094, 0.094, 0.125, 0.042, 0.125, 0.125, and 0.125. The index is calculated by

TABLE 2.1 *The new 2^33^1 design with 12 runs*

A	0	0	1	1	0	0	1	1	0	0	1	1
B	0	1	0	1	0	1	0	1	0	1	0	1
C	0	1	1	0	1	0	0	1	0	1	1	0
U	0	0	0	0	1	1	1	1	2	2	2	2

TABLE 2.2 *The 2^33^1 design with 12 runs (by Webb)*

A	0	0	1	1	0	0	1	1	0	0	1	1
B	0	1	0	1	0	1	0	1	0	1	0	1
C	1	0	0	1	0	1	1	0	0	0	0	1
U	0	0	0	0	1	1	1	1	2	2	2	2

$$\sum_{i=1}^{12} w_i K_i = (0.083 + 0.094 \times 6) + 2/3(0.125 \times 4) + 2(0.042) = 1.062$$

$$I_F = 12/(12 \times 1.062) = 94\%$$

Note that the new design is almost a pairwise orthogonal plan. We have only a small value 0.031 that is caused by different combination of product of ABC in the variance-covariance matrix $(\mathbf{X}^\mathbf{T}\mathbf{X})^{-1}$.

3. THE 2^13^3 DESIGN WITH 18 RUNS

To construct a 3^{3-1} fractional factorial design, we may select a two-degree-of-freedom component of interaction to be a defining contrast. We may choose any component of the ABC interaction to construct the design, that is, ABC, AB^2C, ABC^2, or AB^2C^2. There are twelve distinct 3^{3-1} designs of resolution III defined by

$$A + \alpha_2 B + \alpha_3 C \equiv \delta(mod3) \qquad or \qquad AB^{\alpha_2}C^{\alpha_3} \equiv \delta(mod3)$$

where $\alpha_2, \alpha_3 = 1$ or 2 and $\delta = 0, 1,$ or 2. Note that we use factors and columns interchangeably in this article for convenience.

TABLE 3.1 *The relationship of the transformation*

A	X_{Al}	X_{Aq}		G	X_{Gl}	X_{Gq}
0	-1	1	$\rightarrow$	2	1	1
1	0	-2	$\rightarrow$	1	0	-2
2	1	1	$\rightarrow$	0	-1	1

DEFINITION 3.1. *(By Margolin (1969)) Let Z_1 and Z_2 be two $k \times n$ design matrices for two designs of k runs estimating n effects. These two designs are equivalent if there exists a diagonal $n \times n$ matrix D with main diagonal elements being ± 1, such that $Z_1 = Z_2 D$.*

The estimated parameters for two equivalent designs, $\hat{\beta}_1$ and $\hat{\beta}_2$ are related. It is not hard to show that $\hat{\beta}_1 = \hat{\beta}_2 D$. That is, $\hat{\beta}_{1_i} = \pm\hat{\beta}_{2_i}$ (i=1,2,...,n), and hence the resolution of two equivalent designs should be the same.

Equivalent designs could be obtained by interchanging the low and high levels of any factor. There are six transformation (permutation) of a variable. The above technique is one of them. For example, factor A transform into the new factor G and the relations between these two factors are shown in Table 3.1:

In fact, this kind of transformation is equivalent to transform factor A into factor $G \equiv 2A + 2(\text{mod}3)$. To illustrate the idea, let the design be defined by $A + B + C \equiv 0(\text{mod } 3)$, the transformation B into $2B + 2(\text{mod } 3)$ produces

$$A + (2B + 2) + C \equiv 0(mod\ 3) \qquad or \qquad A + 2B + C \equiv 1(mod\ 3)$$

We obtain that designs $ABC \equiv 0$ and $AB^2C \equiv 1$ are in the same equivalence class. According to the definition, it produces two equivalence classes in the 3^3 fractional factorial design with 9 runs.

(i) $ABC \equiv 0$, $AB^2C \equiv 1$, $ABC^2 \equiv 1$, $AB^2C^2 \equiv 2$.

(ii) $ABC \equiv 1$, $ABC \equiv 2$, $AB^2C \equiv 0$, $AB^2C \equiv 2$, $ABC^2 \equiv 0$, $ABC^2 \equiv 2$, $AB^2C^2 \equiv 0$, $AB^2C^2 \equiv 1$.

Let X_{Al}, X_{Bl}, X_{Cl}, X_{Aq}, X_{Bq}, and X_{Cq} be the orthogonal contrasts defining the corresponding effects. There are some better properties on the first class than the second one. For the first class, we can get Sum(X_{AlBlCl}) = Sum(X_{AlBqCq}) = Sum(X_{AqBlCq}) = Sum(X_{AqBqCl}) = 0. In other words, the vector X_{Al} is orthogonal to the vector X_{BlCl}, for example. Because we want to construct nearly orthogonal designs, the first class will be used to build up the desirable plan.

THEOREM 3.1. *Let two designs be selected from the first class. If we combine these two designs, then the resulting design is an orthogonal main-effect plan with 18 runs that all the main effects and three linear-by-linear interactions can be estimated.*

PROOF. Suppose that two designs $ABC \equiv 0$ and $AB^2C \equiv 1$ are selected. There are some relations in design $ABC \equiv 0$.

$$X_{Aq} - X_{Bq} = 3X_{BlCl} - 3X_{AlCl}, \qquad X_{Aq} - X_{Cq} = 3X_{BlCl} - 3X_{AlBl},$$
$$X_{Bq} - X_{Cq} = 3X_{AlCl} - 3X_{AlBl}.$$

The linear relations of design $AB^2C \equiv 1$ are

$$X_{Aq} - X_{Bq} = -3X_{BlCl} - 3X_{AlCl}, \qquad X_{Aq} - X_{Cq} = -3X_{BlCl} + 3X_{AlBl},$$
$$X_{Bq} - X_{Cq} = 3X_{AlCl} + 3X_{AlBl}.$$

After combining these two designs, the linear relations are broken. Since both designs are orthogonal main-effect plans, the combined design is an orthogonal main-effect plan with 18 runs in which all the main effects and linear-by-linear interactions can be estimated. Similarly, if we choose any two designs from this class, then we will obtain the similar property that the linear relations are broken in the combined design. Finally, the combined design permits estimation of all the main effects and three linear-by-linear interactions. □

Let R be a two-level factor whose levels are R_i, $i = 0$ and 1.

THEOREM 3.2. *If two designs N_1 and N_2 are chosen from the first class, then $N_1R_0 + N_2R_1$ is an orthogonal main-effect plan with 18 runs. In this situation all the main effects and all two-factor interactions involving linear term can be estimated.*

PROOF. The contrast coefficients for the two-level factor are "-1" at its low level, and "+1" at its high level. Let V_1 be the design matrix including the mean, three-level factors, and the interactions between three-level factors. Let V_2 be the design matrix including the two-level factors and the interactions between two- and three-level factors. The matrix $\mathbf{X^TX}$ becomes

$$(V_1 \quad V_2)^T(V_1 \quad V_2) = \begin{bmatrix} V_1^TV_1 & V_1^TV_2 \\ V_2^TV_1 & V_2^TV_2 \end{bmatrix}$$

We obtain $V_2^TV_2$ is a diagonal matrix because of $\text{Sum}(X_{AlR^2}) = \text{Sum}(X_{BlR^2}) = \text{Sum}(X_{ClR^2}) = \text{Sum}(X_{AlBlR}) = \text{Sum}(X_{AlClR}) = \text{Sum}(X_{BlClR}) = 0$. Furthermore, both N_1 and N_2 are orthogonal main-effect plans with $\text{Sum}(X_{AlBlCl}) = 0$, these properties make the submatrix $V_1^TV_2$ to be a zero matrix. By theorem 3.1, $V_1^TV_1$ is a nonsingular submatrix. Hence, this theorem holds.

□

EXAMPLE 3.1. The 2^13^3 design with 18 runs.
The design is constructed by choosing N_1:$AB^2C \equiv 1$, N_2:$ABC^2 \equiv 1$, then $N_1R_0 + N_2R_1$ is an orthogonal main-effect plan and all two-factor interactions involving linear effect can be estimated. Webb chose N_1:$ABC^2 \equiv 0$ and N_1:$ABC^2 \equiv 1$ to construct the design $N_1R_0 + N_2R_1$. This design also provides estimation of all two-factor interactions not involving quadratic term. But there are many complex correlations among estimating effects. The regression model of this design can be written as:

$$E(Y) = \beta_0 + \beta_1X_{Al} + \beta_2X_{Aq} + \beta_3X_{Bl} + \beta_4X_{Bq} + \beta_5X_{Cl} + \beta_6X_{Cq} + \beta_{13}X_{AlBl}$$
$$+\beta_{15}X_{AlCl} + \beta_{35}X_{BlCl} + \beta_7X_R + \beta_{17}X_{AlR} + \beta_{37}X_{BlR} + \beta_{57}X_{ClR}$$

The diagonal elements of $(\mathbf{X^TX})^{-1}$ of Webb's design are: 0.056, 0.094, 0.029, 0.094, 0.029, 0.094, 0.029, 0.167, 0.167, 0.167, 0.056, 0.094, 0.094, and 0.094. The index is calculated by

$\sum_{i=1}^{12} w_iK_i = (0.056\times 2)+(2/3)\times(0.094\times 6)+2(0.029\times 3)+(4/9)\times(0.167\times 3) = 0.885$
$I_F = 14/(18 \times 0.885) = 88\%$

Furthermore, the diagonal entries of $(\mathbf{X^TX})^{-1}$ of the new design are: 0.056, 0.083, 0.056, 0.083, 0.028, 0.083, 0.028, 0.167, 0.167, 0.250, 0.056, 0.083, 0.083, and 0.083. We may obtain the index of the new design

$\sum_{i=1}^{12} w_iK_i = (0.056\times 2)+2/3(0.083\times 6)+2(0.056+0.028\times 2)+(4/9)\times(0.167\times 2+0.250) = 0.926$
$I_F = 14/(18\times 0.926) = 84\%$

Unfortunately, the index of new design (84%) is smaller than the index of Webb's design (88%). However the new design is almost a pairwise orthogonal plan except for a small value (0.083) between the effects $AlBl$ and $AlCl$, or between the effects Aq and $BlCl$ in the matrix $(\mathbf{X}^{\mathbf{T}}\mathbf{X})^{-1}$. Note that if we consider other two designs in the first class, then we will obtain the similar results. For example, suppose that the combined design is obtained by selecting $N_1{:}ABC \equiv 0$, $N_2{:}ABC^2 \equiv 1$, then the index is still 84% and we have a value "-0.083" between the effects $AlBl$ and $BlCl$, or between the effects Bq and $AlCl$ in the matrix $(\mathbf{X}^{\mathbf{T}}\mathbf{X})^{-1}$.

An important example of nonregular design is the 18-run orthogonal array with 7 three-level factors, which has complex aliasing patterns. This design has been constructed by several authors, such as Bose and Bush (1952), Masuyama (1957), and Addelman and Kempthorne (1961). To save space, we only consider the design in Table 4 by Masuyama. We will use this design to obtain an orthogonal main-effect plan with 18 runs that all the main effects and three linear-by-linear interactions can be estimated.

We might let the two-level factor "R" at low level (0) for the first 9 runs and at high level (1) for the second 9 runs. For this design, there is no theoretical tool like defining contrast subgroup to describe the structure of the design. Hence, computer searching is needed for obtaining the desirable design that all interaction terms not involving quadratic terms are estimable. Any three columns in Table 3.2 are considered to form the design. After computer searching, we find that most of them can reach the requirement. Only three cases have the maximum index (88%), columns 1, 3, and 7, columns 2, 5, and 6, or columns 3, 4, and 7. Unfortunately, we have many nonzero off-diagonal elements of $(\mathbf{X}^{\mathbf{T}}\mathbf{X})^{-1}$. That is, there are correlations among the estimating effects.

4. CONCLUSION

In this paper, we provide the general method to obtain the 2^n3^1 and 2^13^3 designs that all main effects are orthogonal to each other and allow the estimation of all two-factor interactions not involving quadratic term. Webb applied ad hoc methods to construct the desirable design. Note that the design we obtain is

TABLE 3.2 *18-run Array (by Masuyama)*

Run	**1**	**2**	**3**	**4**	**5**	**6**	**7**
1	0	0	0	0	0	0	0
2	0	1	1	1	1	1	1
3	0	2	2	2	2	2	2
4	1	0	0	1	1	2	2
5	1	1	1	2	2	0	0
6	1	2	2	0	0	1	1
7	2	0	1	0	2	1	2
8	2	1	2	1	0	2	0
9	2	2	0	2	1	0	1
10	0	0	2	2	1	1	0
11	0	1	0	0	2	2	1
12	0	2	1	1	0	0	2
13	1	0	1	2	0	2	1
14	1	1	2	0	1	0	2
15	1	2	0	1	2	1	0
16	2	0	2	1	2	0	1
17	2	1	0	2	0	1	2
18	2	2	1	0	1	2	0

almost a pairwise orthogonal plan. How to construct more efficient designs is an interesting thing for the researcher. For example, can we construct the designs that all the main effects and two-factor interactions are uncorrelated to estimate in the mixed combined design? Or, how to construct the run efficient designs according to the criterion of degrees of freedom.

If the mixed $2^5 3^1$ design with 24 runs is constructed by choosing $M_1 : I = ABCDE = ABC = DE$, $M_2 : I = ABCDE = -ABC = -DE$, and $M_3 : I = ABD = ACE = BCDE$, then the combined design $M_1U_0 + M_2U_1 + M_3U_2$ provides the estimation of all main effects and all two-factor interactions not involving quadratic term. There are 23 parameters to estimate with 24 runs. This is an orthogonal main effect plan with 24 runs to estimate 23 parameters. How do we derive these kinds of designs in general? These kinds of designs may merit further investigation.

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