

ON THE CONSTRUCTION OF ROBUST RUN ORDERS OF TREATMENTS

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SUMMARY In this paper we consider the problem of sequentially applying v treatments to n experimental units over time or space and where there may be an unknown trend effect which can be expressed as a polynomial function of the order in which the observations are taken. Methods are given for constructing unequally replicated designs which are optimal in the presence of a linear trend as well as methods for constructing equally replicated designs which are optimal in the presence of higher degree polynomial trends.

1. INTRODUCTION

In this paper we consider the problem of allocating v treatments to n experimental units arranged in some time or space order and where there may be some unknown time or spatial trend. We shall assume that the experimental units occur at equally spaced intervals and that the trend effect may be represented as a smooth polynomial function of the positions in which the observations are obtained. Thus if we let d denote some allocation of treatments to experimental units (d shall henceforth be referred to as a design or run order) and let $y = (y_1, \dots, y_n)'$ denote the ordered vector of observations obtained under d , then the model assumed for the data is

$$y_i = \alpha_t + \beta_0 + \beta_1 i + \beta_2 i^2 + \dots + \beta_p i^p + e_i, \quad i = 1, \dots, n, \quad \dots \quad (1.1)$$

where $\alpha_t =$ the effect of treatment t and the e_i 's are independent random error terms having expectation zero and constant variance σ^2 . We note that the least squares estimator $\hat{\alpha}_t - \hat{\alpha}_s$ derived under a given design d and model (1.1) for $\alpha_t - \alpha_s$ must be orthogonal to the trend effect. In view of this, we give the following definition.

Paper received . July 1990 ; revised December 1991.

AMS (1980) subject classification. 62K15,

Key words and phrases. Polynomial trend effect, trend free, A-optimal, MV-optimal.

Definition 1.1. Let $T_x = (1^x, 2^x, \dots, n^x)'$. We say an estimator $t'y = \sum_{i=1}^n t_i y_i$ is p -trend free under model (1.1) if $t'T_x = 0$ for $x = 0, 1, \dots, p$.

Under certain designs, the estimators $\hat{\alpha}_i - \hat{\alpha}_j$ for $\alpha_i - \alpha_j$ derived under d and model (1.1) reduce to the usual least squares estimators for $\alpha_i - \alpha_j$ under the simpler model

$$y_i = \alpha_i + \epsilon_i, \quad i = 1, \dots, n. \quad \dots (1.2)$$

A design that gives least squares estimates for all $\alpha_i - \alpha_j$, $i \neq j$, that are the same under both models (1.1) and (1.2) is said to be balanced for trend or trend free. Cox (1951) was the first to consider the construction of designs balanced for trend. Since then, a number of other authors have considered the problem of constructing trend balanced designs not only in the context of variety trials, but also in the context of factorial and fractional factorial experiments, e.g., see Cheng (1985), Cheng and Jacroux (1988), Coster and Cheng (1988), Coster (1989), Cox (1951, 1952), Daniel and Wilcoxon (1966), Dickinson (1974), Draper and Stoneman (1968), Hill (1960), Jacroux and Saha Ray (1990), Joiner and Campbell (1976) and Phillips (1964, 1968). In this paper we further consider the construction of trend balanced designs. In section 2, we consider the construction of run orders of treatments that are robust against linear trends. Methods are given for constructing optimal linear trend free run orders when treatments are unequally replicated. In section 3, we consider designs that can be obtained by "combining" trend free designs.

2. LINEAR TRENDS

In this section we shall concentrate on the construction of run orders of treatments that are balanced for linear trends. In general, run orders that are balanced for linear trends require fewer observations than run orders that are balanced for higher degree polynomial trends. Phillips (1968) gives a method for constructing 1-trend free run orders when $n = vr$ for some integer r and all treatments are equally replicated. In this section we give methods for constructing "optimal" 1-trend free run orders when $n = vr + q$, $0 < q \leq v - 1$, where $r = [n/v]$ and $[x]$ denotes the integral part of the decimal expansion for $x > 0$. Throughout the sequel, we shall use $1, 2, \dots, v$ to denote the individual treatments used in an experiment and r_{di} to denote the number of experimental units to which treatment i is applied in a given design d , $i = 1, \dots, v$. In a given design d , we shall let A_{di} , $i = 1, \dots, v$, denote the set of actual position numbers in which treatment i is applied to experimental units, i.e., if under d , $A_{d1} = \{1, 3, 7\}$, then treatment one is applied to experimental units occurring in positions 1, 3, and 7.

A design d^* is said to be A-optimal under model (1.1) or model (1.2) if for any other available design d ,

$$\sum_{i=1}^v \sum_{\substack{j=1 \\ j \neq i}}^v \text{var}(\hat{\alpha}_{d^*i} - \hat{\alpha}_{d^*j}) \leq \sum_{i=1}^v \sum_{\substack{j=1 \\ j \neq i}}^v \text{var}(\hat{\alpha}_{di} - \hat{\alpha}_{dj}). \quad \dots (2.1)$$

where $\text{var}(\hat{\alpha}_{di} - \hat{\alpha}_{dj})$ denotes the variance of $\hat{\alpha}_{di} - \hat{\alpha}_{dj}$ under d . A design d^* is said to be MV-optimal under model (1.1) or model (1.2) if for any other available design d ,

$$\max_{i \neq j} \text{var}(\hat{\alpha}_{d^*i} - \hat{\alpha}_{d^*j}) \leq \max_{i \neq j} \text{var}(\hat{\alpha}_{di} - \hat{\alpha}_{dj}). \quad \dots (2.2)$$

Under model (1.2) and a given design d , the least squares estimator $\hat{\alpha}_{di} - \hat{\alpha}_{dj}$ for $\alpha_i - \alpha_j$ is

$$\hat{\alpha}_{di} - \hat{\alpha}_{dj} = \frac{\sum_{p \in A_{di}} y_p / r_{di}}{\sum_{p \in A_{di}} 1 / r_{di}} - \frac{\sum_{q \in A_{dj}} y_q / r_{dj}}{\sum_{q \in A_{dj}} 1 / r_{dj}} \quad \dots (2.3)$$

and

$$\text{var}(\hat{\alpha}_{di} - \hat{\alpha}_{dj}) = \sigma^2(1/r_{di} + 1/r_{dj}).$$

It is easily seen that if $n = vr + q$, then a design d^* is A-optimal under model (1.2) if

$$r_{d^*i} = r \text{ or } r+1 \text{ for } i = 1, \dots, v, \quad \dots (2.4)$$

and a design d is MV-optimal under model (1.2) if

$$(1) \quad \bar{r}_{di} \geq r \text{ for } i = 1, \dots, v \text{ when } 0 \leq q \leq v-2, \quad \dots (2.5)$$

(2) $\bar{r}_{di} = r$ for some i and $\bar{r}_{dj} = r+1$ for all $j = 1, \dots, v, j \neq i$, when $q = v-1$.

As mentioned previously, a design which is A-optimal or MV-optimal under model (1.2) and which is balanced for a linear trend will also be optimal under model (1.1) with the trend polynomial in (1.1) given by $\beta_0 + \beta_1 i$, $i = 1, \dots, n$.

To begin our construction process, we note that the sum of the position numbers in a run order based on n experimental units is $n(n+1)/2$. Also, for $\hat{\alpha}_{di} - \hat{\alpha}_{dj}$ to be 1-trend free for all $i \neq j$ under a given design d , it follows that

$$\sum_{p \in A_{di}} p / r_{di} = \sum_{q \in A_{dj}} q / r_{dj} = a.$$

Hence

$$\sum_{i=1}^v r_{di} a = na = \sum_{i=1}^v \sum_{p \in A_{di}} p = n(n+1)/2$$

and we see that $a = (n+1)/2$. Thus for a given design d to be 1-trend free, the run order must be constructed so that

$$\sum_{p \in A_{di}} p = r_{di} (n+1)/2 \text{ for } i = 1, \dots, v. \quad \dots (2.6)$$

A-optimal designs. To construct A-optimal designs it follows from (2.4), (2.6) and the fact that the left hand side of (2.6) is an integer, that $(n+1)/2$ is an integer, i.e. that n must be odd. We now give a lemma that is useful for our general construction method and that is essentially given in Phillips (1968).

Lemma 2.1. *Suppose $n = 3v$ is odd. Then there exists a run order of treatments $1, \dots, v$ having all treatments replicated 3 times that is 1-trend free.*

Proof. The proof is by construction. To begin, we note that by (2.6), for a design d to be 1-trend free, it must be the case that for $i = 1, \dots, v$,

$$\sum_{p \in A_{di}} p = 3(n+1)/2. \quad \dots (2.7)$$

Now consider the run order d^* obtained by placing treatments $1, 2, \dots, v$ in $A_{d^*1}, \dots, A_{d^*v}$, respectively, where $A_{d^*i} = \{i, 2v - \mu_i, 2v + v_i + 1\}$, $\mu_i \in \{0, 1, \dots, v-1\}$, $v_i \in \{0, 1, \dots, v-1\}$, $\mu_i = 2(i-1) \pmod{v}$ and $v_i = ((v-3)/2 + i) \pmod{v}$. It is now easy to verify that these position assignments satisfy (2.7), hence they yield a 1-trend free run order d^* and we are done.

Using Lemma 2.1, we now give a method for constructing 1-trend free A-optimal designs whenever possible.

Theorem 2.2. *Let $n = vr + q$, $0 \leq q \leq v-1$, $r \geq 2$, be odd. Then there exists a run order d^* of treatments $1, 2, \dots, v$ that is A-optimal and 1-trend free.*

Proof. The proof is by construction. For a design d^* to be A-optimal, it must have all treatments replicated r or $r+1$ times. For $n = vr + q$, $0 \leq q \leq v-1$, assume treatments $1, \dots, v-q$ are replicated r times and treatments $v-q+1, \dots, v$ are replicated $r+1$ times. We now consider two cases.

Case 1 : r even. To construct the run order d^* for this case, use the following procedure :

(1) Take $r/2$ replications of treatments $1, \dots, v-q$, take $(r-2)/2$ replications of treatments $v-q+1, \dots, v$, and assign them to arbitrary places in positions $1, 2, \dots, (v-q)(r/2) + q(r-2)/2$ of the run order.

(2) Take $r/2$ replications of treatments $1, \dots, v-q$, take $(r-2)/2$ replications of treatments $v-q+1, \dots, v$, and assign them to positions $n - (v-q)(r/2) - q(r-2)/2 + 1, \dots, n$ by reversing the order in which they were assigned to positions $1, 2, \dots, (v-q)(r/2) + q(r-2)/2$ (2.8)

(3) Since n is odd and r is even, it follows that q is odd. So take the remaining 3 replications of treatments $v-q+1, \dots, v$ and assign them to the

$3q$ positions $(v-q)(r/2)+q(r-2)/2+1, \dots, n-(v-q)(r/2)-q(r-2)/2$ using the method described in Lemma 2.1 (let q take the place of v in Lemma 2.1).

Case 2 : r odd. To construct the run order d^* in this case, use the following procedure ;

(1) Take $(r-3)/2$ replications of treatments $1, \dots, v-q$, take $(r+1)/2$ replications of treatments $v-q+1, \dots, v$, and assign them to arbitrary places in positions $1, 2, \dots, (v-q)(r-3)/2+q(r+1)/2$.

(2) Take $(r-3)/2$ replications of treatments $1, \dots, v-q$, take $(r+1)/2$ replications of treatments $v-q+1, \dots, v$, and assign them to positions $n-(v-q)(r-3)/2-q(r+1)/2+1, \dots, n$ by reversing the order in which they were assigned to positions $1, 2, \dots, (v-q)(r-3)/2+q(r+1)/2$ (2.9)

(3) Since n is odd and r is odd, it follows that $v-q$ is odd. So take the remaining 3 replications of treatments $1, \dots, v-q$ and assign them to the $3(v-q)$ positions $(v-q)(r-3)/2+q(r+1)/2+1, \dots, n-(v-q)(r-3)/2-q(r+1)/2$ using the method described in Lemma 2.1 (let q take the place of v in Lemma 2.1).

It is now easily verified that for both run orders d^* constructed using (2.8) and (2.9), for treatment i ,

$$\sum_{p \in \Delta_{d^*}^i} p = \begin{cases} r(n+1)/2 & \text{for } 1 \leq i \leq v-q, \\ (r+1)(n+1)/2 & \text{for } v-q+1 \leq i \leq v, \end{cases}$$

and we have the desired result.

MV-optimal designs. From (3.4) and (2.5), we see that a design that is A-optimal under model (1.2) is also MV-optimal. Thus if possible, it is desirable to construct an A-optimal design. But to construct an A-optimal design based on n experimental units that is also 1-trend free, we saw earlier that n must be odd. However, when n is even, though an A-optimal 1-trend free run order is impossible to obtain, we can still in many situations construct an MV-optimal run order that is 1-trend free.

Theorem 2.3. *Let $n = vr + q$, $0 \leq q \leq v-2$, where r and q are both even. Then there exists a run order d^* of treatments $1, \dots, v$ that is MV-optimal and 1-trend free.*

Proof. For a design d^* to be MV-optimal under model (1.2), we see from (2.5) that d^* must have $r_{d^*i} \geq r$ for $i = 1, \dots, v$. Also from (2.6), it follows that for any run order to be 1-trend free, all treatments must have an even

number of replications. To construct the required run order d^* under the conditions given, we proceed as follows:

(1) Take $r/2$ replications of treatments $1, \dots, v-(q/2)$ and $(r+2)/2$ replications of treatments $v-(q/2)+1, \dots, v$ and assign these replications arbitrarily to experimental units occurring in positions $1, 2, \dots, (v-(q/2))(r/2) + (q/2)(r+2)/2$ (2.10)

(2) Take $r/2$ replications of treatments $1, \dots, v-(q/2)$ and $(r+2)/2$ replications of treatments $v-(q/2)+1, \dots, v$ and assign treatments to experimental units occurring in positions $(v-(q/2))(r/2) + (q/2)(r+2)/2 + 1, \dots, n$ by reversing the order in which treatments were assigned to positions $1, 2, \dots, (v-(q/2))(r/2) + (q/2)(r+2)/2$.

It is now easily seen that for treatment i ,

$$\sum_{p \in A_{d^*}^i} p = \begin{cases} r(n+1)/2 & \text{for } i = 1, \dots, v-(q/2), \\ (r+2)(n+1)/2 & \text{for } i = v-(q/2)+1, \dots, v. \end{cases}$$

Hence we have the desired result.

Comment. The only values of n for which there is no 1-trend free A-or MV-optimal design are those values of n which are even and for which r is odd or r and q are both even with $q = v-1$. The reason for the former is, of course, that when r is odd, at least one treatment must be replicated r times. But then $r(n+1)/2$ is not an integer and (2.6) cannot be satisfied. Also, when r and q are both even with $q = v-1$, an MV-optimal design d^* must have $r_{d^*i} = r$ for some i and $r_{d^*j} = r+1$ for $j = 1, \dots, v, j \neq i$. Thus in this case an MV-optimal design is also A-optimal by (2.4) and an A-optimal design is impossible to construct when n is even as we saw earlier.

3. COMBINING DESIGNS

In this section we consider the problem of obtaining new trend free run orders of treatments from existing trend free run orders. With this in mind, we give a useful lemma.

Lemma 3.1. Suppose $\hat{\alpha}_{d_1i} - \hat{\alpha}_{d_1j}$ is p_1 -trend free in run order d_1 based on n_1 experimental units and $\hat{\alpha}_{d_2i} - \hat{\alpha}_{d_2j}$ is p_2 -trend free in run order d_2 based on n_2 experimental units $p_1 \leq p_2$.

(a) If $r_{d_1i} = r_{d_1j}$ and $r_{d_2i} = r_{d_2j}$, then $\hat{\alpha}_{d_1i} - \hat{\alpha}_{d_1j}$ is at least p_1 -trend free in $d = (d_1, d_2)$.

(b) If $r_{d_1i} = r_{d_2i}$ and $r_{d_1j} = r_{d_2j}$, then $\alpha_{d_1} - \alpha_{d_2}$ is at least p_1 -trend free in $d = (d_1, d_2)$.

Proof. (a) Using (2.3) and the fact that $r_{d_1i} = r_{d_1j}$, and $r_{d_2i} = r_{d_2j}$, it is easy to verify

$$\begin{aligned} \sum_{l \in A_{d_1i}} l^x &= \sum_{l \in A_{d_1j}} l^x \text{ for } x = 0, \dots, p_1, \\ \sum_{l \in A_{d_2i}} l^x &= \sum_{l \in A_{d_2j}} l^x \text{ for } x = 0, \dots, p_2. \end{aligned} \quad \dots (3.1)$$

Thus, from (3.1), we see that for $x = 0, \dots, p_1$,

$$\begin{aligned} \sum_{l \in A_{d_1i}} l^x + \sum_{l \in A_{d_2i}} (n_1 + l)^x &= \sum_{l \in A_{d_1i}} l^x + \sum_{l \in A_{d_2i}} \left\{ \sum_{s=0}^x \binom{x}{s} n_1^{x-s} l^s \right\} \\ &= \sum_{l \in A_{d_1i}} l^x + \sum_{s=0}^x \binom{x}{s} n_1^{x-s} \left\{ \sum_{l \in A_{d_2i}} l^s \right\} \\ &= \sum_{l \in A_{d_1j}} l^x + \sum_{s=0}^x \binom{x}{s} n_1^{x-s} \left\{ \sum_{l \in A_{d_2j}} l^s \right\} \\ &= \sum_{l \in A_{d_1j}} l^x + \sum_{l \in A_{d_2j}} \sum_{s=0}^x \binom{x}{s} n_1^{x-s} l^s \\ &= \sum_{l \in A_{d_1j}} l^x + \sum_{l \in A_{d_2j}} (n_1 + l)^x. \end{aligned}$$

From this last expression and the fact that $r_{d_1i} = r_{d_1j}$ and $r_{d_2i} = r_{d_2j}$, we obtain the desired result.

(b) From (2.3), it follows that

$$\begin{aligned} \sum_{l \in A_{d_1i}} l^x / r_{d_1i} &= \sum_{l \in A_{d_1j}} l^x / r_{d_1j} \text{ for } x = 0, 1, \dots, p_1, \\ \sum_{l \in A_{d_2i}} l^x / r_{d_2i} &= \sum_{l \in A_{d_2j}} l^x / r_{d_2j} \text{ for } x = 0, 1, \dots, p_2. \end{aligned} \quad \dots (3.2)$$

Thus, since $r_{d_1i} = r_{d_2i}$ and $r_{d_1j} = r_{d_2j}$ and from (3.2), we see that for $x = 0, 1, \dots, p_1$,

$$\begin{aligned} \sum_{l \in A_{di}} l^x / r_{di} &= \left\{ \sum_{l \in A_{d_1i}} l^x + \sum_{l \in A_{d_2i}} (n_1 + l)^x \right\} / 2r_{d_1i} \\ &= (1/2) \left\{ \sum_{l \in A_{d_1i}} l^x + \sum_{l \in A_{d_2j}} \sum_{s=0}^x \binom{x}{s} n_1^{x-s} l^s \right\} / r_{d_1i} \end{aligned}$$

$$\begin{aligned}
&= (1/2) \left\{ \sum_{l \in A_{d_1}} l^x / r_{d_1 l} + \sum_{s=0}^x \binom{x}{s} n_1^{x-s} \sum_{l \in A_{d_2}} l^s / r_{d_2 l} \right\} \\
&= (1/2) \left\{ \sum_{l \in A_{d_1}} l^x + \sum_{l \in A_{d_2}} \sum_{s=0}^x \binom{x}{s} n_1^{x-s} l^s \right\} / r_{d_1 l} \\
&= \left\{ \sum_{l \in A_{d_1}} l^x + \sum_{l \in A_{d_2}} (n_1 + l)^x \right\} / 2r_{d_1 l} = \sum_{l \in A_{d_1}} l^x / r_{d_1 l}
\end{aligned}$$

from which the desired result follows.

Corollary 3.2. *Suppose d_1 is a p_1 -trend free run order of treatments and d_2 is a p_2 -trend free run order of treatments, $p_1 \leq p_2$.*

(a) *If $r_{d_1 1} = \dots = r_{d_1 v}$ and $r_{d_2 1} = \dots = r_{d_2 v}$, then $d = (d_1, d_2)$ is at least p_1 -trend free.*

(b) *If $r_{d_1 i} = r_{d_2 i}$ for $i = 1, \dots, v$, then $d = (d_1, d_2)$ is at least p_1 -trend free.*

We note that if the conditions of Corollary 3.2 do not hold, then an estimator for $\alpha_1 - \alpha_j$ that is obtained from $d = (d_1, d_2)$ may not be p_1 -trend free.

Example 3.3. Let $d_1 = (121)$ and $d_2 = (212)$. Then

$$\hat{\alpha}_{d_1 1} - \hat{\alpha}_{d_1 2} = (y_1 + y_2)/2 - y_2 \text{ and } \hat{\alpha}_{d_2 1} - \hat{\alpha}_{d_2 2} = y_2 - (y_1 + y_2)/2$$

are both 1-trend free. However, for design $d = (d_1, d_2) = (121212)$, the estimator $\hat{\alpha}_{d 1} - \hat{\alpha}_{d 2} = (y_1 + y_2 + y_6)/3 - (y_3 + y_4 + y_5)/3$ is not 1-trend free.

Using Corollary 3.2 as a basis, it is possible to construct certain designs that have a specified degree of minimal trend resistance.

Theorem 3.4. *Suppose $n = v^t p \geq 2v$ where $p = fv + q$, $0 \leq q \leq v - 1$.*

(a) *If $t = 1$, v is even and p is odd, then there does not exist an equally replicated run order of treatments that is even 1-trend free.*

(b) *If $t = 1$ and v and p do not satisfy the conditions given in (a), then there exists an equally replicated run order of treatments that is at least 1-trend free.*

(c) *If $t \geq 2$ and p is even, then there exists an equally replicated run order of treatments that is at least t -trend free.*

(d) *If $t \geq 2$, $f = 0$ and p is odd, then there exists an equally replicated run order of treatments that is at least $(t-1)$ -trend free. If in addition, $f \geq 1$ and q or $v+q$ is even, then there exists an equally replicated run order of treatments that is at least t -trend free.*

Proof. Parts (a) and (b) essentially follow from the results given in Phillips (1968).

(c) We can write

$$n = v^t p = (2v^t) (p/2) \quad \dots \quad (3.3)$$

Using the results of Jacroux and Saha Ray (1990), it follows that there exists a design \bar{d}_0 based on $2v^t$ experimental units that is t -trend free. Thus, by Corollary 3.2, it follows that $d = (d_1, \dots, d_{p/2})$ is t -trend free where $d_i = \bar{d}_0$ for $i = 1, \dots, p/2$.

(d) If $t \geq 2$ and p is odd, it follows from the results of Jacroux and Saha Ray (1990) that there exists a design \bar{d}_0 based on v^t experimental units which is $(t-1)$ -trend free and has all treatments replicated v^{t-1} times each. It now follows from Corollary 3.2 that $d = (d_1, \dots, d_p)$ where $d_i = \bar{d}_0$ for $i = 1, \dots, p = q$ is at least $(t-1)$ -trend free.

If $f \geq 1$ and q is even, we can write

$$n = v^t(fv+q) = fv^{t+1} + (q/2)(2v^t) \quad \dots \quad (3.4)$$

or when $f \geq 1$ and $v+q$ is even, we can write

$$n = v^t(fv+q) = (f-1)v^{t+1} + ((v+q)/2)(2v^t). \quad \dots \quad (3.5)$$

In either case, it follows from the results of Jacroux and Saha Ray (1990) that we can find a design \bar{d}_0 based on v^{t+1} experimental units which is t -trend free and a design \bar{d}_1 based on $2v^t$ experimental units which is also t -trend free. Thus, if $f \geq 1$, q is even and we write n as in (3.4), then it follows from Corollary 3.2 that $d = (d_1, \dots, d_{f+(q/2)})$ is at least t -trend free where $d_i = \bar{d}_0$ for $i = 1, \dots, f$ and $d_i = \bar{d}_1$ for $i = f+1, \dots, f+q/2$. Also, if $f \geq 1$, $v+q$ is even and we write n as in (3.5), then it follows from Corollary 3.2 that $d = (d_1, \dots, d_{f-1+(v+q)/2})$ is at least t -trend free where $d_i = \bar{d}_0$ for $i = 1, \dots, f-1$ and $d_i = \bar{d}_1$ for $i = f, \dots, (f-1)+(v+q)/2$.

Comment. Since all the designs d constructed in Theorem 3.4 for $t \geq 2$ have all treatments equally replicated, it follows from (2.4) that all these designs are A-optimal under both models (1.1) and (1.2) (assuming the appropriate degree of polynomial trend is used in (1.1)).

Comment. In the proofs of Theorem 3.4 (c) and (d), the subdesigns d_i used to make up d do not have to occur in the order specified. In fact, the designs d_i can be put in any order and still have Theorem 3.4 hold.

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