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Optimality Results of 3^m Fractional Factorial Designs for $N \equiv p$ mod 9 Runs, $p = 1, 2, 3$.

Fotini Kolyva-Machera and Stavros A. Chatzopoulos
Department of Mathematics, Aristotle University, 54124, Thessaloniki, Greece.

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Abstract

The optimality of fractional factorial designs for $N \equiv p$ mod 9 runs, $p = 1, 2, 3$, is studied, when an experiment involves m factors each at three levels. The optimality criterion used here, is the Φ-optimality employing the notion of majorization. Unlike what happens with orthogonal array plus one run plans, the behavior of plans obtained via augmentation of an orthogonal array by two or three runs depends on the particular runs added.

Key words: Fractional factorial; Orthogonal array; Majorization; Φ-, E-, A-, D-optimality.

1. Introduction

The problem of finding optimal experimental designs for any number N of runs and under different optimality criteria, preoccupies researchers working in this area, almost six decades. Although there are hundreds of papers on 2^m fractional factorial designs (f.f.d. for short), there are few papers on 3^m f.f.d. The extension of theorems concerning 2^m f.f.d. to the 3^m f.f.d. is not evident, since the elements of the design matrix of a 2^m f.f.d. are ± 1, fact which is not valid for the case of 3^m f.f.d. and generally for s^m f.f.d. It is well known that in general s^m setup, when the number of runs is $N \equiv 0$ mod s^2 the corresponding information matrix is diagonal and the optimal designs are constructed via orthogonal arrays (OA for short), Hedayat *et al.* (1999), Raghavarao (1971). For $N \not\equiv 0$ mod s^2, $s > 2$, the problem of finding optimal f.f.d. is partially solved in Chai *et al.* (2002), Chatzopoulos *et al.* (2011), Kolyva-Machera (1989a), Kolyva-Machera (1989b), Mukerjee *et al.* (1999), Pericleous *et al.* (2017) where the authors found the type 1 optimal designs for s^m f.f.d. in the class of O.A. plus p runs. A wide list of optimal f.f.d. can be found in Dey and Mukerjee (1999). In this paper we give Φ-optimal designs for $N \equiv p$ mod 9 runs, $p = 1, 2, 3$ using the notion of majorization.

The paper is organized as follows. The notations and preliminaries are presented in section 2, while section 3 deals with the main results of this paper. Our findings are illustrated with examples in section 4.

Corresponding Author: Fotini Kolyva-Machera
E-mail: fkolyva@math.auth.gr
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2. Notations and Preliminaries

Consider a factorial experiment involving $m\ (\geq 2)$ factors $F_1, \ldots, F_m$ each at 3 levels, coded $0, 1, 2$. A typical level combination of the factors is denoted as $\ell_1\ell_2\cdots\ell_m$, where $\ell_j = 0, 1, 2$, $j = 1, 2, \ldots, m$. Let $\mathcal{D}_N$ be the class of designs with $N \equiv p$ mod 9 runs, $p = 1, 2, 3$, consisting of the treatment combinations $\ell_{i1}\ell_{i2}\cdots\ell_{im}$, where $i = 1, 2, \ldots, N$, $j = 1, 2, \ldots, m$, $\ell_{ij} = 0, 1, 2$. For any positive integer t, let $\mathbf{1}_t$ be the $t \times 1$ vector with all elements unity and $\mathbf{I}_t$ (or simply $\mathbf{I}$ if there is no risk for confusion) be the identity matrix of order t and $\mathbf{P} = \begin{pmatrix} \mathbf{p}(0) & \mathbf{p}(1) & \mathbf{p}(2) \end{pmatrix}$ be a 2×3 matrix satisfying

$$\mathbf{PP}' = 3\mathbf{I}_2, \quad \mathbf{P1}_3 = \mathbf{0}, \quad \mathbf{p}'(k)\mathbf{p}(l) = 3\delta_{k\ell} - 1, \quad k, \ell = 0, 1, 2, \tag{2.1}$$

where $\mathbf{0}$ is a null vector of an appropriate order, $\mathbf{P}'$ denotes the transpose of matrix $\mathbf{P}$ and $\delta_{k\ell}$ is the Kronecker delta. So, the 2×3 matrix $\mathbf{P}$ satisfying (2.1) is

$$\mathbf{P} = \begin{pmatrix} -\sqrt{\frac{3}{2}} & 0 & \sqrt{\frac{3}{2}} \\ \sqrt{\frac{1}{2}} & -2\sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} \end{pmatrix}. \tag{2.2}$$

Let $\mathbf{z}_j$ (or $\mathbf{z}_{jN}$, if needed), $1 \leq j \leq m$ be an $N \times 2$ matrix with rows $\mathbf{p}'(0)$ or $\mathbf{p}'(1)$ or $\mathbf{p}'(2)$ and θ_j be the vector of main effect parameters of factor F_j. Then under the assumption of the absence of interaction effects involving two or more factors, we have the following linear model

$$\left.\begin{array}{lcl} E(\mathbf{Y}) & = & \mathbf{1}_N\mu + \sum_{j=1}^{m} z_j\theta_j, \\ Var(\mathbf{Y}) & = & \sigma^2\mathbf{I}_N, \end{array}\right\} \tag{2.3}$$

where $\mathbf{Y}$ is the $N \times 1$ vector of observations (response).

Define the design matrix $\mathbf{R} = [\mathbf{1}_N, z_1, \cdots, z_m]$. The information matrix of a design $d \in \mathcal{D}_N$ will then be

$$\mathbf{M}_N = \mathbf{R}'\mathbf{R}. \tag{2.4}$$

2.1 Properties of the Information Matrix

Consider two subsets of a design $d \in \mathcal{D}_N$ with $N_1 < N$ and $N_2 = N - N_1$ runs, respectively. For $\ell = 1, 2$ let $\mathbf{z}_{jN_\ell}$ be the $N_\ell \times 2$ matrix with rows $\mathbf{p}(a_{ij})\mathbf{p}'(a_{ij})$, $1 \leq i \leq N_\ell$, $1 \leq j \leq m$ and $N_1 + N_2 = N$. Then:

$$\mathbf{R} = \begin{pmatrix} \mathbf{R}_1 \\ \mathbf{R}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{1}_{N_1} & z_{1N_1} & z_{2N_1} & \ldots & z_{mN_1} \\ \mathbf{1}_{N_2} & z_{1N_2} & z_{2N_2} & \ldots & z_{mN_2} \end{pmatrix} \tag{2.5}$$

and the information matrix of any design $d \in \mathcal{D}_N$ can be written as:

$$\mathbf{M}_N = \mathbf{R}_1'\mathbf{R}_1 + \mathbf{R}_2'\mathbf{R}_2 = \mathbf{M}_1 + \mathbf{M}_2, \tag{2.6}$$

that is $\mathbf{M}_N$ can be decomposed in two (or more) information matrices with N_1 and $N_2 = N - N_1$ runs, respectively.

Remark 2.1. If $\mathbf{M}_1 = N_1\mathbf{I}$, then $N_1 \equiv 0$ mod 9 and the off-diagonal elements of the information matrix $\mathbf{M}_2$ are equal to the off-diagonal elements of the information matrix $\mathbf{M}_N$, while the diagonal elements of $\mathbf{M}_2$ are equal to the diagonal elements of $\mathbf{M}_N$ minus N_1.

Definition 2.1. *For $i \neq j = 1, 2, \ldots, m$, $\ell, k = 0, 1, 2$, let $n_i(\ell)$ be the number of runs where the ith factor enters the experiment at level ℓ and $n_{ij}(\ell k)$ be the number of runs where the i-th factor enters the experiment at level ℓ and j-th factor enters the experiment at level k. It holds that*

$$\begin{array}{ll} N = \sum_{\ell=0}^{2} n_i(\ell), & N = \sum_{\ell=0}^{2}\sum_{k=0}^{2} n_{ij}(\ell k), \\ n_i(\ell) = \sum_{k=0}^{2} n_{ij}(\ell k), & n_j(k) = \sum_{\ell=0}^{2} n_{ij}(\ell k). \end{array} \tag{2.7}$$

The information matrix of a design $d \in \mathcal{D}_N$, for the model (2.3), after some simple matrix manipulations, using the parametrization (2.2) can be written as:

$$\mathbf{M}_N = \begin{pmatrix} N & \sqrt{\frac{3}{2}}\mathbf{a}' & \sqrt{\frac{1}{2}}\mathbf{b}' \\ \sqrt{\frac{3}{2}}\mathbf{a} & \frac{3}{2}\mathbf{A} & \frac{\sqrt{3}}{2}\mathbf{C} \\ \sqrt{\frac{1}{2}}\mathbf{b} & \frac{\sqrt{3}}{2}\mathbf{C}' & \frac{1}{2}\mathbf{B} \end{pmatrix}, \tag{2.8}$$

where **a**, **b** are $m \times 1$ vectors , **A** and **B** are $m \times m$ symmetric matrices and **C** is an $m \times m$ matrix. For $i \neq j = 1, 2, \ldots, m$ the elements of the above vectors and matrices are given by the following relations:

$$\begin{array}{ll} a_i = n_i(2) - n_i(0), & b_i = N - 3n_i(1), \\ a_{ii} = N - n_i(1), & a_{ij} = n_{ij}(00) + n_{ij}(22) - n_{ij}(02) - n_{ij}(20), \\ b_{ii} = N + 3n_i(1), & b_{ij} = N - 3n_i(1) - 3n_j(1) + 9n_{ij}(11), \\ c_{ii} = n_i(2) - n_i(0), & c_{ij} = n_i(2) - n_i(0) + 3[n_{ij}(01) - n_{ij}(21)]. \end{array} \tag{2.9}$$

Remark 2.2. From relationships (2.9) it is obvious that trace($\mathbf{M}_N$) $= N + \sum_{i=1}^{m}(\frac{3}{2}a_{ii} + \frac{1}{2}b_{ii}) = (2m+1)N$.

Lemma 2.1. *Let $U_1 = \{a_i, b_i, a_{ii}, b_{ii}, c_{ii}\}$ and $U_2 = \{a_{ij}, b_{ij}, c_{ij}, c_{ji}\}$, $i \neq j = 1, 2, \ldots, m$. The elements of these two sets are all even or all odd.*

Proof. After a simple algebra, using (2.7) and (2.9), for $i \neq j = 1, 2, \ldots, m$, one can easily verify the following relationships:

$$a_i + b_i = 2(n_i(2) - n_i(1)) = 2\widetilde{a}_i. \tag{2.10}$$

$$a_{ii} + b_{ii} + 2c_{ii} = 4(N - n_i(0)) = 4\widetilde{a}_{ii}. \tag{2.11}$$

$$a_{ij} + c_{ij} = 2[n_{ij}(01) + n_{ij}(22) - n_{ij}(02) - n_{ij}(21)]. \tag{2.12}$$

$$a_{ij} + b_{ij} = 2[-n_i(1) - n_j(1) + n_{ij}(00) + n_{ij}(22) + 4n_{ij}(11)]. \tag{2.13}$$

$$c_{ji} + b_{ij} = 2[n_j(2) - n_j(1) + 3n_{ij}(11) - 3n_{ij}(12)] = 2\widetilde{c}_{ji}. \tag{2.14}$$

$$a_{ij} + c_{ij} + c_{ji} + b_{ij} = 4[n_{ij}(11) + n_{ij}(22) - n_{ij}(12) - n_{ij}(21)] = 4\widetilde{a}_{ij}. \tag{2.15}$$

$$c_{ii} + b_{ii} = 2[2n_i(1) + n_i(2)] = 2\widetilde{c}_{ii}. \tag{2.16}$$

From (2.10)-(2.16) the proof of lemma is obvious. □ □

Lemma 2.2. *It holds that* $det(\boldsymbol{M}_N) = 3^{3m}z$, $z \in \mathbb{Z}$.

Proof. Let us denote:

$$\widetilde{\mathbf{M}}_N = \begin{pmatrix} N & \mathbf{a}' & \mathbf{b}' \\ \mathbf{a} & \mathbf{A} & \mathbf{C} \\ \mathbf{b} & \mathbf{C}' & \mathbf{B} \end{pmatrix}. \tag{2.17}$$

Then, from (2.8) we have:

$$det(\mathbf{M}_N) = \frac{3^m}{2^{2m}} det(\widetilde{\mathbf{M}}_N). \tag{2.18}$$

By adding the $(m+1+j)$-th rows and columns to the $(j+1)$-th rows and columns, $j = 1, 2, \ldots, m$, respectively, from (2.17), we get that:

$$det(\widetilde{\mathbf{M}}_N) = det \begin{pmatrix} N & \mathbf{a}' + \mathbf{b}' & \mathbf{b}' \\ \mathbf{a} + \mathbf{b} & \mathbf{A} + \mathbf{C} + \mathbf{C}' + \mathbf{B} & \mathbf{C} + \mathbf{B} \\ \mathbf{b} & \mathbf{C}' + \mathbf{B} & \mathbf{B} \end{pmatrix},$$

that is from (2.10), (2.11), (2.13)-(2.16), we have:

$$det(\widetilde{\mathbf{M}}_N) = 2^{2m} det \begin{pmatrix} N & \widetilde{\mathbf{a}}' & \mathbf{b}' \\ \widetilde{\mathbf{a}} & \widetilde{\mathbf{A}} & \widetilde{\mathbf{C}} \\ \mathbf{b} & \widetilde{\mathbf{C}}' & \mathbf{B} \end{pmatrix},$$

where for $i \neq j = 1, 2, \ldots, m$ the elements of $m \times m$ matrices $\widetilde{\mathbf{A}} = (\widetilde{a}_{ij})$ and $\widetilde{\mathbf{C}} = (\widetilde{c}_{ij})$ are as defined in (2.11), (2.15) and (2.14), (2.16), respectively, while the elements of the $m \times 1$ vector $\widetilde{\mathbf{a}}$ are given in (2.10). By subtracting the first row and column from the $(m+1+j)$-th, $j = 1, 2, \ldots, m$, rows and columns, respectively, we have:

$$det(\widetilde{\mathbf{M}}_N) = 2^{2m} det \begin{pmatrix} N & \widetilde{\mathbf{a}}' & \mathbf{b}' - N\mathbf{1}_m' \\ \widetilde{\mathbf{a}} & \widetilde{\mathbf{A}} & \widetilde{\mathbf{C}} - \widetilde{\mathbf{a}}\mathbf{1}_m' \\ \mathbf{b} - N\mathbf{1}_m & \widetilde{\mathbf{C}}' - \mathbf{1}_m\widetilde{\mathbf{a}}' & \mathbf{B} - \mathbf{b}\mathbf{1}_m' - \mathbf{1}_m\mathbf{b}' + N\mathbf{1}_m\mathbf{1}_m' \end{pmatrix}.$$

It can be easily seen that:

$$b_i - N = -3n_i(1). \tag{2.19}$$

$$\widetilde{c}_{ii} - \widetilde{a}_i = 3n_i(1). \tag{2.20}$$

$$\widetilde{c}_{ji} - \widetilde{a}_j = 3(n_{ij}(11) - n_{ij}(12). \tag{2.21}$$

$$\widetilde{b}_{ii} - 2\widetilde{b}_i + N = 9n_i(1). \tag{2.22}$$

$$\widetilde{b}_{ji} - \widetilde{b}_i - \widetilde{b}_j + N = 9n_{ji}(11). \tag{2.23}$$

Using (2.19)-(2.23), we get

$$det(\widetilde{\mathbf{M}}_N) = 3^{2m}2^{2m} det \begin{pmatrix} N & \widetilde{\mathbf{a}}' & \widetilde{\mathbf{b}}' \\ \widetilde{\mathbf{a}} & \widetilde{\mathbf{A}} & \widetilde{\mathbf{E}} \\ \widetilde{\mathbf{b}} & \widetilde{\mathbf{E}}' & \widetilde{\mathbf{B}} \end{pmatrix}, \tag{2.24}$$

where $\widetilde{\mathbf{b}}$ is a $m \times 1$ vector, $\widetilde{\mathbf{B}}$ is a $m \times m$ symmetric matrix and $\widetilde{\mathbf{E}}$ is a $m \times m$ matrix. For $i \neq j = 1, 2, \ldots, m$ the elements of the above vectors and matrices are given by the following relations:

$$\begin{aligned} &\widetilde{b}_i = -n_i(1), \\ &\widetilde{b}_{ii} = n_i(1), \quad \widetilde{b}_{ij} = n_{ij}(11), \\ &\widetilde{e}_{ii} = n_i(1), \quad \widetilde{e}_{ij} = n_{ij}(11) - n_{ij}(21). \end{aligned}$$

□

From relations (2.18) and (2.24) the result follows. □

2.2 Optimality and Majorization

Definition 2.2. *A design $d^* \in \mathcal{D}_N$, with information matrix M_N^*, is said to be Φ-optimal if it minimizes a functional Φ of the information matrix $\boldsymbol{M}_N$ of any design $d \in \mathcal{D}_N$, that is, $\Phi(\boldsymbol{M}_N) \geq \Phi(\boldsymbol{M}_N^*)$. In other words, d^* minimizes $\phi(\lambda_1)+\phi(\lambda_2)+\ldots+\phi(\lambda_k)$ for all continuous, decreasing and convex functions $\phi(\lambda)$ (Marshall* et al. *(1979), p.11), where λ_i, $i = 1, 2, \ldots, k$ are the latent roots of the information matrix $\boldsymbol{M}_N$. Note that A-, E-, D-optimality are special cases of Φ-optimality. Consideration of the functions $\phi(\boldsymbol{M}) = log\{det(\boldsymbol{M}^{-1})\}$, $\phi(\boldsymbol{M})$ =trace$(\boldsymbol{M}^{-1})$ and $\phi(\boldsymbol{M})$ largest eigenvalue of $\boldsymbol{M}^{-1}$, which are all members of Φ, shows that a Φ-optimal plan is also D-,A-, and E-optimal.*

The following definition 2.3 can be found in Marshall *et al.* (1979), p.7, p.11.

Definition 2.3. *If $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^k$, $\boldsymbol{x} = (x_1, x_2, \ldots, x_k)'$, $\boldsymbol{y} = (y_1, y_2, \ldots, y_k)'$, then $\boldsymbol{x}$ is majorized by $\boldsymbol{y}$ ($\boldsymbol{x} \prec \boldsymbol{y}$) if $x_{(1)} + x_{(2)} + \ldots + x_{(j)} \geq y_{(1)} + y_{(2)} + \ldots + y_{(j)}$, $j = 1, 2, \ldots, k-1$ and $x_{(1)} + x_{(2)} + \ldots + x_{(k)} = y_{(1)} + y_{(2)} + \ldots + y_{(k)}$.*

Lemma 2.3. *The following lemma can be found in (Marshall* et al. *(1979), p.11). For majorization the following conditions are equivalent:*

(a) $\boldsymbol{x} \prec \boldsymbol{y}$.

(b) $\sum_{i=1}^{k} \phi(x_i) \leq \sum_{i=1}^{k} \phi(y_i)$ *for all continuous convex functions* ϕ.

An immediate consequence of lemma 2.3 is the following lemma 2.4.

Lemma 2.4. *A design d^* with $k \times k$ information matrix $\boldsymbol{M}_N^*$ and latent roots $\lambda_1, \lambda_2, \ldots, \lambda_k$, is Φ-optimal in the class $\mathcal{D}_N$ of designs, if the latent roots of $\boldsymbol{M}_N^*$ are majorized by the latent roots of the information matrix $\boldsymbol{M}_N$ of any design $d \in \mathcal{D}_N$.*

Lemma 2.5. *Let $\boldsymbol{Q}$ be a positive definite matrix of order k (pd(k), for short) and $\lambda(\boldsymbol{Q})$ the vector of the latent roots of $\boldsymbol{Q}$. For the completely symmetric matrix $\boldsymbol{Q}^* = (a^* - b^*)I_k + b^* J_k$, where a^* is the mean of the diagonal elements of $\boldsymbol{Q}$ and b^* is the mean of the off diagonal elements of Q, it holds $\lambda(\boldsymbol{Q}^*) \prec \lambda(\boldsymbol{Q})$.*

Proof. See Kiefer (1975). □ □

Lemma 2.6. *If $\boldsymbol{Q} = (q_{ij})$ is a pd(k) matrix with vector of diagonal elements $\delta(\boldsymbol{Q}) = (q_{11}, q_{22}, \ldots, q_{kk})'$ and vector of latent roots $\lambda(\boldsymbol{Q}) = (\lambda_1, \lambda_2, \ldots, \lambda_k)'$, then $\delta(\boldsymbol{Q})$ is majorized by $\lambda(\boldsymbol{Q})$. Equality holds only iff $\boldsymbol{Q}$ is diagonal.*

Proof. See Pukelsheim (1993), p.146. □ □

Lemma 2.7. *If s_1: $x_1 = x_2 = \ldots = x_k = x$, s_2: $y_1, y_2, \ldots, y_k$ not all equal and $y_1+y_2+\ldots+y_k = kx$, then $(x_1, x_2, \ldots, x_k)$ is majorized by $(y_1, y_2, \ldots, y_k)$ or $s_1 \prec s_2$.*

Proof. See Pericleous *et al.* (2017). □ □

Corollary 2.1. *An immediate consequence of lemmas 2.2, 2.4 and 2.7 is that the design d^* with information matrix $\boldsymbol{M}_N^* = N\boldsymbol{I}_k$ is Φ-optimal. However, $\boldsymbol{M}_N^* = \boldsymbol{R}'\boldsymbol{R} = N\boldsymbol{I}_k$, which means that the columns of $\boldsymbol{R}$ are orthogonal.* □

3. Main Results

Let us now consider a $(2m+1)\times(2m+1)$ information matrix $\mathbf{M}_N$ with constant trace$(\mathbf{M}_N) = (2m+1)N$ and latent roots $\lambda_1, \lambda_2, \ldots, \lambda_{2m+1}$. Without loss of generality we may assume that $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_{2m+1}$. If we denote

$$S_v = (\frac{1}{v}\sum_{i=1}^{v}\lambda_i, \ldots, \frac{1}{v}\sum_{i=1}^{v}\lambda_i, \lambda_{v+1}, \ldots, \lambda_{2m+1}) \tag{3.1}$$

then from definition 2.3 we have $s_1 \succ s_2 \succ \ldots \succ s_{2m+1}$. Moreover, let us denote

$$S_{vu} = (\frac{1}{v}\sum_{i=1}^{v}\lambda_i, \ldots, \frac{1}{v}\sum_{i=1}^{v}\lambda_i, \frac{1}{u}\sum_{i=1}^{u}\lambda_{v+i}, \ldots, \frac{1}{u}\sum_{i=1}^{u}\lambda_{v+i}, \lambda_{v+u+1}, \ldots, \lambda_{2m+1}) \tag{3.2}$$

that is S_{vu} has v components equal to $\frac{1}{v}\sum_{i=1}^{v}\lambda_i$, u components equal to $\frac{1}{u}\sum_{i=1}^{u}\lambda_{v+1}$ and the $(2m+1-v-u)$ components $(\lambda_{v+u+1}, \ldots, \lambda_{2m+1})$. Then, if $S_v = S_{v1}$, from definition 2.3 it holds that $S_v \succ S_{v2} \succ \ldots \succ S_{v(2m+1-u)}$. In what follows $\mathbf{M}_{S_v}$ is the information matrix with latent roots as defined in (3.1) and $\mathbf{M}_{S_{vu}}$ is the information matrix with latent roots as defined in (3.2). Then from lemma 2.3 it holds that:

$$\Phi(\mathbf{M}_N) = \Phi(\mathbf{M}_{S_1}) \geq \Phi(\mathbf{M}_{S_2}) \geq \ldots \geq \Phi(\mathbf{M}_{S_{2m+1}}) \tag{3.3}$$

and for $v = 1, 2, \ldots, 2m$ we have

$$\Phi(\mathbf{M}_{S_v}) \geq \Phi(\mathbf{M}_{S_{v1}}) \geq \ldots \geq \Phi(\mathbf{M}_{S_{v(2m+1-u)}}). \tag{3.4}$$

The information matrix $\mathbf{M}_{S_{2m+1}}$ has $2m+1$ equal latent roots $\lambda_i = N$, $i = 1, 2, \ldots, 2m+1$, minimizes $\Phi(\mathbf{M}_N)$, so the design $d^* \in \mathcal{D}_N$ is Φ-optimal. From relations (2.9), the information matrix M_N, given in (2.8), is diagonal iff $n_i(0) = n_i(1) = n_i(2) = N/3$, $i = 1, 2, \ldots, m$ and $n_{ij}(\ell k) = N/9$, $i \neq j = 1, 2, \ldots, m$, which is true iff $N \equiv 0$ mod 9, and d^* is given by an $OA(N, m, 3, 2)$.

Remark 3.1. For $N \not\equiv 0$ mod 9, the information matrix of the Φ-optimal design $d^* \in \mathcal{D}_N$, from (3.3) and (3.4) will be $\mathbf{M}_{S_{v(2m+1-v)}}$, $v < 2m+1$, with v, as close to $2m+1$ as possible. Also, matrix $\mathbf{M}_{S_{v(2m+1-v)}}$ has v latent roots equal to $\lambda < N$, and u latent roots equal to $\lambda_i' = (2m+1)\frac{N-\lambda}{u} + \lambda$, $v + u = 2m + 1$.

Lemma 3.1. *Consider an s^m f.f.d. where $s \geq 3$. Let $1 \leq p \leq s+1$ and $\mathcal{D}_{OA}$ be the class of designs obtained by adding p runs to an OA and $\boldsymbol{M}_{OA}$ be the corresponding information matrix of a design $d \in \mathcal{D}_{OA}$. This design is E-optimal in the class $\mathcal{D}_{OA}$.*

Proof. See [Dey and Mukerjee (1999), p.111]. □

Lemma 3.2. *The information matrix $\boldsymbol{M}_{OA}$ has $2m+1-p$ latent roots equal to $N-p$ and p latent roots $\lambda_i > N-p$, $i = 1, \ldots, p$.*

Proof. See [Chatzopoulos *et al.* (2011), lemma 3]. □

From definition 2.2, design $d \in \mathcal{D}_{OA}$, with information matrix $\mathbf{M}_{OA}$, is E-optimal if d maximizes the smallest eignvalue of $\mathbf{M}_{OA}$. If $\lambda(\mathbf{M}_{OA}) = (\mu_1, \mu_2, \ldots, \mu_{2m+1})$, then from lemmas 3.1 and 3.2, $(\mu_1, \mu_2, \ldots, \mu_{2m+1}) = (N-p, \ldots, N-p, \lambda_1, \lambda_2, \ldots, \lambda_p)$ with $\lambda_i > N-p$, $i = 1, 2, \ldots, p$. So, it holds that maxmin$\{\mu_1, \mu_2, \ldots, \mu_{2m+1}\} = N - p$,

Theorem 3.1. *Let $d^* \in \mathcal{D}_N$ be the Φ-optimal design with information matrix M^*. If $N \equiv p$ mod 9, $p \neq 0$, then for the smallest latent root of M^* it holds that $\lambda = N - p$.*

Proof. As E-optimality is a special case of Φ-optimaity and $\mathcal{D}_{OA} \subset \mathcal{D}_N$, for the maximum of the smallest latent root of the Φ-optimal design $d^* \in \mathcal{D}_N$, it holds that $N - p \leq \lambda < N$, where $N \equiv p$ mod 9. On the other hand, from lemma 2.2, for any information matrix $\mathbf{M}_N$ of a 3^m f.f.d, it holds that det$(\mathbf{M}_N) = 3^{3m}z$, $z \in \mathbb{Z}$, that is, if $\mathbf{M}_N^* = \mathbf{M}_{S_{v(2m+1-v)}}$, then

$$det(\mathbf{M}_N^*) = \lambda^v(\lambda + (2m+1))\frac{N-\lambda}{u}))^u = 3^{3m}z, \tag{3.5}$$

where $z \in \mathbb{Z}$, $v + u = 2m + 1$ and v as close to $2m + 1$ as possible, or u as small as possible. For $N - \lambda \leq p \leq 3$, relation 3.5 holds for $\lambda = N - p$. □

Lemma 3.3. *If a pd(q) matrix $\boldsymbol{M}$ has latent roots: λ with multiplicity $q - k$, $q > k$ and $\lambda_1, \lambda_2, \ldots, \lambda_k$, where $\lambda < \lambda_i$, $1 \leq i \leq k$, then this matrix can be written as $\boldsymbol{M} = \lambda\boldsymbol{I} + \boldsymbol{F}\boldsymbol{F}'$, where $\boldsymbol{F}$ is a $q \times k$ matrix.*

Proof. For any pd(q) matrix $\mathbf{M}$ exists an orthogonal $q \times q$ matrix $\mathbf{W}$, where $\mathbf{W}\mathbf{W}' = \mathbf{I}_q$, such that $\mathbf{W}'\mathbf{M}\mathbf{W} = \mathbf{D}$, where $\mathbf{D}$ is a $q \times q$ diagonal matrix. If $\mathbf{M}$ has latent roots: λ with multiplicity $q - k$, $q > k$ and $\lambda_1, \lambda_2, \ldots, \lambda_k$, where $\lambda < \lambda_i$, $1 \leq i \leq k$, then $\mathbf{D} = \begin{pmatrix} \mathbf{V} & \mathbf{0} \\ \mathbf{0} & \lambda\mathbf{I}_{q-k} \end{pmatrix}$, where $\mathbf{V} = diag(\lambda_1, \lambda_2, \ldots, \lambda_k)$ or $\mathbf{D} = \lambda\mathbf{I}_q + \begin{pmatrix} \mathbf{V} - \lambda\mathbf{I}_k & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$. Then

$$\mathbf{M} = \mathbf{W}\mathbf{D}\mathbf{W}' = \lambda\mathbf{I}_q + \mathbf{W}\begin{pmatrix} \mathbf{V} - \lambda\mathbf{I}_k & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}\mathbf{W}',$$

that is

$$\mathbf{M} = \lambda \mathbf{I}_q + (\mathbf{W}_1 \quad \mathbf{W}_2) \begin{pmatrix} \mathbf{V} - \lambda \mathbf{I}_k & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{W}_1' \\ \mathbf{W}_2' \end{pmatrix},$$

or

$$\mathbf{M} = \lambda \mathbf{I}_q + \mathbf{W}_1(\mathbf{V} - \lambda \mathbf{I}_k)\mathbf{W}_1' = \lambda \mathbf{I}_q + \mathbf{F}\mathbf{F}',$$

where $\mathbf{F} = \mathbf{W}_1(\mathbf{V}^{1/2} - \sqrt{\lambda}\mathbf{I}_k)$.□ □

As $\mathcal{D}_{OA} \subset \mathcal{D}_N$, we will try to find a design $d^* \in \mathcal{D}_N$ with information matrix $\mathbf{M}_N^*$, such that $\lambda(\mathbf{M}_N^*) \prec \lambda(\mathbf{M}_{OA}^*)$.

Lemma 3.4. *It holds that $\boldsymbol{M}_{S_v} = (N-p)\boldsymbol{I} + \boldsymbol{M}_p$, where $\boldsymbol{M}_p$ is an information matrix such that $\boldsymbol{M}_p = \boldsymbol{R}_1'\boldsymbol{R}_1$ and $\boldsymbol{R}_1'$ is a $(2m+1) \times p$ design matrix.*

Proof. From relation (3.1), theorem 3.1 and lemma 3.3 it holds that $\lambda = N - p$ and $\mathbf{M}_{S_v} = (N-p)\mathbf{I}_q + \mathbf{F}\mathbf{F}'$. Matrix $\mathbf{F}\mathbf{F}'$ has off-diagonal elements the off-diagonal elements of matrix $\mathbf{M}_{S_v}$ and diagonal elements the diagonal elements of matrix $\mathbf{M}_{S_v}$ minus $N-p$. From remark 2.1 matrix $\mathbf{F}\mathbf{F}'$ is an information matrix, say $\mathbf{M}_p$ of a design with p runs and the result follows. □ □

Lemma 3.5. *For $p = 1, 2, 3$ and $w = 1, 2$, let $\boldsymbol{x} = (x_{(1)}, x_{(2)}, \ldots, x_{(p)})$, where $x_{(1)} = g - w(p-1)$, $x_{(i)} = g + w$, $i = 2, 3, \ldots, p$, $\boldsymbol{z} = (z_{(1)}, z_{(2)}, \ldots, z_{(p)})$, where $z_{(p)} = g - (p-1)(w-3)$, $z_{(i)} = g + w - 3$, $i = 1, 2, \ldots, p-1$ and $\sum_{i=1}^{p} z_{(i)} = \sum_{i=1}^{p} x_{(i)} = pg$. Then:*

(i) $\boldsymbol{z} \prec \boldsymbol{x}$ *for* $w = 2$.

(ii) $\boldsymbol{x} \prec \boldsymbol{z}$ *for* $w = 1$.

Proof. Since $\sum_{i=1}^{p} z_{(i)} = \sum_{i=1}^{p} x_{(i)}$, from definition 2.2 we have that:

(i) If $w = 2$ then

$$\begin{aligned} \mathbf{z} \prec \mathbf{x} &\Leftrightarrow \sum_{i=1}^{j} z_{(i)} \geq \sum_{i=1}^{j} x_{(i)}, j = 1, 2, \ldots, p-1 \Leftrightarrow \\ &\Leftrightarrow j(g-1) \geq j(g+2) - 2p, j = 1, 2, \ldots, p-1 \Leftrightarrow \\ &\Leftrightarrow 2p \geq 3j, j = 1, 2, \ldots, p-1, \end{aligned}$$

which is true beacuse $p = 1, 2, 3$, that is $2p \geq 3(p-1) \geq 3j$, $j = 1, \ldots, p-1$.

(ii) If $w = 1$ then

$$\begin{aligned} \mathbf{x} \prec \mathbf{z} &\Leftrightarrow \sum_{i=1}^{j} z_{(i)} \leq \sum_{i=1}^{j} x_{(i)}, j = 1, 2, \ldots, p-1 \Leftrightarrow \\ &\Leftrightarrow (g-2)j \leq j(g+1) - p, j = 1, 2, \ldots, p-1 \Leftrightarrow \\ &\Leftrightarrow p \leq 3j, j = 1, 2, \ldots, p-1. \end{aligned}$$

□ □

Theorem 3.2. *Suppose that the* $OA(N-p, m, 3, 2)$ *exists for some* p, $p = 1, 2, 3$ *and let* $\mathcal{D}_{OA}$ *be the class of designs obtained by adding* p *runs to an* $OA(N-p, m, 3, 2)$. *Let* $d^* \in \mathcal{D}_{OA}$ *be the* Φ*-optimal design in this class and* $\mathbf{M}^*_{OA} \in \mathcal{M}_{2m+1}$ *is the corresponding information matrix. The latent roots of* $\mathbf{M}^*_{OA}$ *are* $N-p$ *with multiplicity* $2m+1-p$, $N-p+2m+1-y$ *with multiplicity* $p-1$ *and* $N-p+2m+1+(p-1)y$ *with multiplicity 1, where* $y = 3m_1^* - m + 1$ *with* m_1^* =*round*$[(m-1)/3]$, *and round*$[t]$ *is the nearest integer to* t.

Proof. From relation (2.5) and (2.6) and remark 2.1 we have $\mathbf{M}_{OA} = (N-p)\mathbf{I}_{2m+1} + \mathbf{R}_1'\mathbf{R}_1$, with $\mathbf{R}_1 = (1_p, z_{1p}, z_{2p}, \ldots, z_{mp})$, where z_{jp}, $1 \le j \le m$ are $p \times 2$ matrices as defined in section 2. The latent roots of matrix $\mathbf{M}_{OA}$ are $N-p$ with multiplicity $2m+1-p$ and the latent roots of the $p \times p$ matrix $\mathbf{Q} = (N-p)\mathbf{I}_p + \mathbf{R}_1\mathbf{R}_1'$ (say $\lambda_1, \lambda_2, \ldots, \lambda_p$). From Chai *et al.* (2002) and Chatzopoulos *et al.* (2011), the diagonal elements of $\mathbf{R}_1\mathbf{R}_1'$ are $2m+1$ and the off-diagonal elements are $3m_{ij} - m + 1$, $1 \le i \ne j \le p$, where m_{ij} is the number of coincidences between level combinations $\ell_{i1}\ell_{i2}\cdots\ell_{im}$ and $\ell_{j1}\ell_{j2}\cdots\ell_{jm}$. Then, $Tr((N-p)\mathbf{I}_p + \mathbf{R}_1\mathbf{R}_1') = p(N-p+2m+1)$, which is independent of the design d.

Let us now consider the matrix $\mathbf{Q}^*$ with diagonal elements the mean of the diagonal elements of $\mathbf{Q}$ and off-diagonal elements the mean of the off-diagonal elements of $\mathbf{Q}$. If we denote $a = N-p+2m+1$ and $b = 3m_1 - m + 1$, where m_1 is the mean number of coincidences between the level combinations $\ell_{i1}\ell_{i2}\cdots\ell_{im}$ and $\ell_{j1}\ell_{j2}\cdots\ell_{jm}$, $1 \le i \ne j \le p$, then $\mathbf{Q}^* = (a-b)\mathbf{I}_p + b\mathbf{J}_p$. The latent roots of $\mathbf{Q}^*$ are $a-b$ with multiplicity $p-1$ and $a-b+pb$ with multiplicity one. From lemma 2.5 we have $\lambda(\mathbf{Q}^*) \prec \lambda(\mathbf{Q}))$ and from lemma 2.3 we get $\Phi(\mathbf{Q}) \ge \Phi(\mathbf{Q}^*)$.

It holds that:

$$\Phi(\mathbf{M}_{OA}) = (2m+1-p)\phi(N-p) + \sum_{i=1}^{p}\phi(\lambda_i) =$$

$$= (2m+1-p)\phi(N-p) + \Phi(\mathbf{Q}) \ \ge (2m+1-p)\phi(N-p) + \Phi(\mathbf{Q}^*) =$$

$$= (2m+1-p)\phi(N-p) + (p-1)\phi(N-p+2m+1-(3m_1-m+1)) + \\ +\phi(N-p+2m+1+(p-1)(3m_1-m+1)) \ge$$

$$\ge (2m+1-p)\phi(N-p) + (p-1)\phi(N-p+2m+1-(3m_1^*-m+1)) + \\ +\phi(N-p+2m+1+(p-1)(3m_1^*-m+1)) = \phi(\mathbf{M}^*_{OA}),$$

where m_1^* is the mean value of coincidences minimizing $g(m_1) = (p-1)\phi((N-p+2m+1-(3m_1-m+1)) + \phi(N-p+2m+1+(p-1)(3m_1-m+1))$.

Indeed, if $m-1 \equiv 0\text{mod}3$, then for $m_1 = (m-1)/3$, matrix Q^* is diagonal and $Q^* = (N-p+2m+1)I_p$.

If $(m-1) = 3c+w$, $c \in \mathbb{Z}$, $1 \le w \le 2$, then $3m_1 - (m-1) = 3(m_1-c) - w$, that is $c < (m-1)/3 < c+1$. Consequently, for $m_1 = c$ we have $3m_1 - (m_1-1) = -w$, while for $m_1 = c+1$ we have $3m_1 - (m_1-1) = 3-w$ and the corresponding vectors of the latent roots are **x** and **z**, respectively, as defined in lemmma 3.5 for $g = N-p+2m+1$. Moreover, from lemmma 3.5, if $m \not\equiv 1$ mod 3, then m_1 should be the nearest integer to $(m-1)/3$, that is m_1^* =round$[(m-1)/3]$ for $p = 1, 2, 3$. □ □

Theorem 3.3. *Consider an 3^m fractional factorial design and the class of designs $\mathcal{D}_N$ with $N \equiv p$ mod 9 runs, $p = 1, 2, 3$, and that $OA(N-p, m, 3, 2)$ exists. Let also consider the p level combinations $\ell_{j1}\ell_{j2}\cdots\ell_{jm}$, $j = 1, 2, \ldots, p$, such that any two level combinations have an equal number m_1^* =round$[(m-1)/3]$ of coincidences. The design $d^* \in \mathcal{D}_N$ obtained by adding the above p level combinations to an $OA(N-p, m, 3, 2)$ is Φ-optimal*

Proof. From relation (3.1) the Φ-optimal design is the one having information matrix $\mathbf{M}_{s_{2m+1}} = N\mathbf{I}_{2m+1}$ which implies that the design is orthogonal and $N \equiv 0$ mod 9. For $N \equiv p$ mod 9, $p \neq 0$, the optimal design, should have information matrix $\mathbf{M}_{s_v}$, $\mathbf{M}_{s_v} \in \mathcal{M}_{2m+1}$, with $v \leq 2m$ as great as possible. Since M_{s_v} has v equal latent roots λ, from lemma 3.4, we have that matrix $\mathbf{M}_{s_v}$ is decomposed in two information matrices, such that $\mathbf{M}_{s_v} = (N-p)\mathbf{I}_{2m+1} + \mathbf{R}_1'\mathbf{R}_1$. As mentioned in theorem 3.2, the multiplicity of eigenvalue $N-p$ is $v = 2m+1-p$ (the greatest possible). So, from theorem 3.1, we have $\mathbf{M}_{s_v} = \mathbf{M}_{OA}$. Consequently, for any design $d \in \mathcal{D}_N$, with information matrix $\mathbf{M}_N$, $\mathbf{M}_N \in \mathcal{M}_{2m+1}$, from theorems 3.1 and 3.2, it holds:

$$\begin{aligned} \Phi(\mathbf{M}_N) = \Phi(\mathbf{M}_{s_1}) \geq \Phi(\mathbf{M}_{s_v}) = \Phi(\mathbf{M}_{OA}) \geq \\ \geq (2m+1-p)\phi(N-p) + (p-1)\phi(N-p+2m+1-(3m_1^*-m+1)) + \\ +\phi(N-p+2m+1+(p-1)(3m_1^*-m+1)) = \Phi(\mathbf{M}_{d^*}), \end{aligned}$$

where m_1^* =round$[(m-1)/3]$. Hence, the design $d^* \in \mathcal{D}_N$ obtained as described in the statement of theorem 3.3 is Φ-optimal. □ □

The following examples clarify our main results.

4. Examples

For $N \equiv 1$ mod s^2 and $k = (s-1)m+1$, we have from theorem 3.3 that $\Phi(\mathbf{M}_N) \geq (k-1)\phi(N-1) + \phi(N-p+k)$. The information matrix of a design obtained by adding any run to an $OA(N-1, m, s, 2)$ is $\mathbf{M}_{OA}^* = (N-1)\mathbf{I}_k + \mathbf{f}\mathbf{f}'$, where $\mathbf{f}'$ is any row of matrix $\mathbf{R}$ as defined in (2.4). The latent roots of $\mathbf{M}_{OA}^*$ are, $N-1$ with multiplicity $k-1$ and $1+\mathbf{f}'((N-1)\mathbf{I}_k)^{-1}\mathbf{f} = (N-1+k)$, according to lemma 2.1. So, this design is Φ-optimal. Kolyva-Machera (1989a), Kolyva-Machera (1989b) proved that the design obtained by adding any run to an $OA(N-1, m, 3, 2)$ is D- and G-optimal. Also, Mukerjee *et al.* (1999) proved that the design obtained by adding any run to an $OA(N-1, m, s, 2)$ is type 1 optimal. Note that type 1 optimality includes D-, A- and E-optimality (see Cheng (1978)).

For $N \equiv p$ mod 9 runs, $p = 2, 3$, a Φ-optimal 3^m f.f.d. can be founded by adding p of the following level combinations: $\ell_{11}\ell_{12}\ldots\ell_{1m}, \ell_{21}\ell_{22}\ldots\ell_{2m}, \ell_{31}$ $\ell_{32}\ldots\ell_{3m}$, where for $h \neq i \neq k \neq h$ $\ell_{hj} \neq \ell_{ij} \neq \ell_{kj} \neq \ell_{hj}$, for $j = 1, 2, \ldots, m - m_1^*$ and $\ell_{ij} = \ell_{kj} = \ell_{hj}$, for $j = m - m_1^* + 1, \ldots, m$ to an $OA(N-p, m, 3, 2)$.

Conclusion. The problem of finding optimal fractional factorial designs for any $N \not\equiv 0$ mod s^2, $s > 2$ has stuck for many years. Although this paper solves the problem, the existence of orthogonal arrays for any $N \equiv 0$ mod s^2 and any m, is necessary and the problem of finding optimal designs, remains open for futher research.

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