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The Concept of Majorization in Experimental Designs

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Abstract. The information of interest is contained in the variance matrix, $\mathbf{V} = \sigma^2\mathbf{Q}^{-1}$, or equivalently in the information matrix $\mathbf{Q}$. The problem of finding estimators minimizing a decreasing convex functional of the variance matrix or maximizing an increasing concave functional of the information matrix is crucial in statistics. There are several optimality criteria in bibliography. We explain how the concept of Majorization can be used to investigate optimal experimental designs.

Keywords: Majorization, direct effects, carry-over effects, universally optimality, F-Optimality, repeated measurements designs, saturated designs, row-column, factorial designs

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The concept of universally optimal designs was given by Kiefer (1975 a), who generalized the idea of a Balanced Block Design (BBD) and showed when the GYD is universally optimal. Also he worked on their construction (Kiefer, 1975 b) and generalized the results of the work of Agrawal (1966), Hartley and Smith (1948), Shrikhande (1951).

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Bibliography on finding and constructing universally optimal designs and optimal designs satisfying some criteria are quite extensive. Interesting is the case of two treatments with independent observations and with even number of units (Kounias and Chalikias 2008a, 2015; Chalikias and Kounias 2012, 2017). In contrast, the bibliography on cases of three or more treatments is limited (Chalikias 2017). This happens because when the number of treatments is $v \geq 3$, the theoretical and computational aspects demand a different approach.

In this paper the row designs with homogeneous populations under dependence will be investigated especially the Balance Block Designs and the row-column designs with two and three treatments and depended observations are mentioned. Moreover we will examine the comparisons of v treatments with a standard treatment under dependence.

Kiefer (1975 a) introduced a new method to generalize the existing results. An improved approach on the same subject is given in the book by F. Pukelsheim (1993).

Many researchers worked with problems of optimal designs using the model with dependent observations, such as Chauhan (2000), Chauhan and Martin (2001), Kunert (1988), Martin and Eccleston (1993), Morgan and Uddin (1991), Uddin (1997), Uddin and Morgan (1991).

Optimal row-column designs when the treatments are two with positive dependence between the observations have been examined by Morgan and Uddin (2002).

Pericleous and Kounias (2010) worked in finding universally optimal designs comparing v treatments with a standard (control) treatment. We examined cases where experimental units are homogeneous or heterogeneous with one characteristic. The concept of mazorization was applied and the universally optimal design was presented when the population is homogeneous. In heterogeneous populations Pericleous and Kounias first applied the concept of mazorization and then found A-, D- and MV-optimal designs.

The definitions of information function and information matrix were given in (Pericleous and Kounias, 2011), in the line followed by Pukelsheim (1993). The definitions of information function and information matrix are given. Homogeneous populations set in a row with dependent observations are examined and properties of the optimal designs are presented, two treatments are studied in more detail and the optimal designs are given. Non homogeneous populations by one characteristic set in p rows and q columns, with independent observations, are analyzed and examples of Balanced Treatments Block designs are given.

Row designs are examined (Pericleous and Kounias 2012) with three treatments, homogeneous population with dependent observations. The dependence follows a first order autoregression (AR(1)). A filtering procedure was presented to reduce the number of competing designs.

In the case of optimal designs in 3^k fractional factorial for the estimating linear and quadratic contrasts, most of the works for constructing optimal designs for parameter estimation in fractional factorials are concentrated in factors at two levels. It is of interested estimating linear and quadratic contrasts, in fractional factorials, with each factor at three levels. The books by Dey and Mukerjee (1999) and Wu and Hamada (2000), cover the topic, with a lot references. If the number of runs is N=0mod9, the orthogonal arrays, OA(N; k; 3; 2), are Φ-optimal under different type of criteria, Kiefer(1958, 1960). If N=1mod9 the plan obtained by augmentation of a run to an OA(N -1; k; 3; 2) is D-optimal, Kolyva-Machera (1989a), G-optimal, Kolyva-Machera(1989b), and optimal under Cheng's type 1 criteria, Mukerjee (1999). These efforts were concentrated in adding runs to an OA(N; k; 3; 2) so that the resulting design is optimal in some sense.

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In this project we will deal with factorial designs with factors, each at 3 levels, the primary interest is the estimation of linear and quadratic contrasts of factor's effects. Orthogonal designs, called orthogonal balanced arrays (OBA), are derived for any value of the number of experimental runs, in which the estimators of linear contrasts are uncorrelated with those of quadratic contrasts.

Another issue of interesting in experimental designs is saturated designs. An experimental design is said to be saturated if all degrees of freedom are consumed by the estimation of parameters, leaving no degrees of freedom for error variance estimation. Saturated resolution III factorial designs are commonly used in screening experiments, to determine which of many factors affects the measure of pertinent quality characteristics. The purpose of this paper is to give saturated resolution III designs, minimizing the generalized variance of the main effects and the general mean, that is, D-optimal designs. In recent years, there has been a considerable interest in optimal saturated main effect designs. Mukerjee et al. (1986) and Kraft (1990) showed that in the two-factor case all such designs are equivalent with respect to D-optimality. Later Mukerjee and Sinha (1990) considered optimality results on almost saturated main effect designs in the two-factor case. The result was also obtained by Pesotan and Raktoe (1988) in the special case of 2^mfactorials, who also worked on a subclass of 3^mfactorials. The first attempt to extend the two factor results to three factors was done by Chatterjee and Mukerjee (1993). Later Chatterjee and Narasimhan (2002) using techniques from Graph Theory and Combinatorics, claimed about the upper bound of the determinant of the saturated $3 x m_2 x m_3$ factorials. Chatzopoulos and Machera (2002) considered the class of $m_1 \times m_2 \times m_3$, $m_1 \geq 2$, $m_2 \geq m_1$, $m_3 \geq m_2$ factorial plans with the minimum number of observations. Their interest was to find conditions in order to maximize the determinant of the information matrix and compare their findings with other researchers' findings. Chatzopoulos and Kolyva-Machera (2005), considered the problem of finding an algorithm in order to construct D-optimal saturated factorial designs with three factors. The interest was to estimate the general mean and main effects while all higher order interactions are negligible, that is Resolution III plans. In order to reduce the steps of the algorithm, they diminish the number of the cases and have to search by studying the design matrix. The algorithm they suggested, leads in finding the upper bound of the determinant of the design and moreover in constructing the D-optimal design. They apply an algorithm in order to find the D-optimal saturated $4\times 4\times m_3$, $m_3 \geq 6$ design and compare their results with those are mentioned in bibliography. Moreover they verify the findings for the $4 \times 4 \times 4$ and $4 \times 4 \times 5$ D-optimal saturated designs and expand their results by applying the algorithm for the saturated $4 \times 5 \times 5$ and $4 \times 5 \times 6$ designs. Moreover, Chatzopoulos and Kolyva-Macher (2006) extended the results concerning D-optimal saturated main effect designs for $2\times m_2\times m_3$ to $3\times m_2\times m_3$ factorials, when $3 \leq m_2 \geq 6$ and $m_3 \geq m_2$. Recently Karagiannis and Moyssiadis (2005, 2008) extended the above cases and studied the D-optimal $3\times m_2\times m_2$ and $3\times m_2\times(m_2+1)$ saturated designs.

Although the issue has been studied by many researchers it is not exhausted. This area of research is far from complete because of the difficulty of the calculations for designs that are not symmetrical. Optimal designs are found only in certain cases.

2 Majorization

The information of interest is contained in the variance matrix, $\mathbf{V} = \sigma^2\mathbf{Q}^{-1}$, or equivalently in the information matrix $\mathbf{Q}$. There are several optimality criteria in bibliography. The most frequently used optimality criteria are:

G–optimality: If $E(y_i) = f'(\mathbf{x}_i)\theta,\ \ f(\mathbf{x}_i) = (f_1(\mathbf{x}_i),...,f_p(\mathbf{x}_i))',\ \ i = 1,...,n$ is the linear model, then the variance response surface in points $\mathbf{x}_i,\ \ i = 1,...,n$, is $\operatorname{var}(f'(x_i)\hat{\theta}) = \sigma^2 f'(x_i)\mathbf{V}f(x_i)$ and for G-optimality: $\min_d \max_i f'(\mathbf{x}_i)\mathbf{V}f(\mathbf{x}_i)$.

G-optimality criterion is "a prediction criterion". This criterion latterly is called global or G–optimality. The aim of G-optimality is a response estimation criterion and can be defined as minimizing the maximum variance of any predicted value over the experimental space.

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D–optimality is a quite popular criterion maximizing the determinant of the information matrix, in essence D-optimality chooses that design as the "best" for which the volume (expected volume) of the joint confidence ellipsoid of the parameters of interest is minimized.

A-optimality: $\min_d(\text{trace}\,\mathbf{V}_d)$ *or* $\max_d(\text{trace }\ \mathbf{Q}_d^{-1})^{-1}$.

A-optimality is defined as minimizing the average variance of the parameter estimates, that is, minimizing the average variance of the best linear unbiased estimator (BLUE) of the parameters of interest.

E-optimality: $\min_d \max_i \lambda_i(\mathbf{V})$ or $\underbrace{\max}_d \underbrace{\min}_i \lambda_i(\mathbf{Q})$.

E–optimality is defined as maximizing the minimum eigenvalue of the information matrix or equivalently, minimizing the maximum eigenvalue of the inverse of the information matrix. The aim of E-optimality is to minimize the maximum variance of all possible normalized linear combinations of parameter estimates.

MV-optimality: $\min_d \max_i (v_{ii}), \quad \mathbf{V} = (v_{ij})$.

MV–optimality is defined as minimizing the maximum variance of the parameters of interest.

Instead of dealing with specific optimality criteria is preferable to work with universal optimality, an idea introduced by Kiefer (1975), and Φ-optimality and if such designs do not exist, then go to the specific criteria mentioned above.

Universal and Φ-optimality are defined below:

Definition 1: If $C \in nnd(k)$ the function $\varphi(\mathbf{C})$ is called information function if $\varphi(\mathbf{C}) \to \mathbb{R}$, and the following conditions are satisfied:

(i) $\mathbf{C} \geq \mathbf{D} \Rightarrow \varphi(\mathbf{C}) \geq \varphi(\mathbf{D})$

(ii) $\varphi(p\mathbf{C} + (1-p)\mathbf{D}) \geq p\varphi(\mathbf{C}) + (1-p)\varphi(\mathbf{D}) \qquad \forall\ 0 < p < 1,\ \mathbf{C}, \mathbf{D} \geq \mathbf{0}$

(iii) $\varphi(dC) = d\varphi(C), \quad \forall\ d > 0,\ \mathbf{C} \geq \mathbf{0} \Rightarrow \varphi(\mathbf{0}) = 0 \Rightarrow \varphi(\mathbf{C}) \geq 0\ ,\ \forall\ \mathbf{C} \geq \mathbf{0}$

(iv) $\varphi(\mathbf{C}) = \varphi(\mathbf{PCP}') \ \ \forall\ \mathbf{C} \in nnd(k),\ \ \mathbf{P} \in perm(k)$

So the information functions are concave and increasing. Here $nnd(k)$ is for non negative definite $k \times k$ matrix, perm(k) is for permutation $k \times k$ matrix.

Definition 2: A design d^* with information matrix $\mathbf{C}_d^*$ is universally optimal, in the class F of designs, if it maximizes $\varphi(\mathbf{C}_d),\ d \in F$, for all information functions φ .

Definition 3: A design d^* with information matrix $\mathbf{C}_d^*$ is Φ-optimal, in the class F of designs, if $\sum_{i=1}^{v} \varphi\left(\lambda_i\right) \leq \sum_{i=1}^{v} \varphi\left(\mu_i\right)$ for all continuous, decreasing convex functions φ, where $\lambda = (\lambda_1, \ldots, \lambda_v)$ are the latent roots of $\mathbf{C}_d^*$ and $\mu = (\mu_1, \ldots, \mu_v)$ are the latent roots of $C_d \ \ \forall\ \ d \in F$.

This is equivalent to: $\lambda \prec \mu$, that is, the vector λ is majorized by the vector μ (Marshall and Olkin p.10).

If a design is universally optimal it is also Φ-optimal and if a design is Φ-optimal, it is A-, D-, E-optimal. Also a design may be optimal for a criterion but not optimal for the other criteria. Note that MV-optimality is not covered by Φ-optimality, since it cannot be expressed as a function of the latent roots of the information matrix.

The idea is to use the concept of majorization in order to establish Φ optimality.

3 Fields of Applications

They will be present in three fields of application of the concept of majorization, one for each different case of experimental designs.

1) The first idea is for Repeated measurements of p periods, two treatments, 2^p sequences (we use the symbolism $s_i \ \ i = 0,1,\ldots,m,$ where $m = 2^p - 1$).

For the estimation of the parameters we have:

If n is the total number of experimental units and $u_i \ \ i = 0,1,\ldots,m$ is the number of experimental units that the sequence s_i of treatments is applied, then $u_0 + u_1 + \ldots + u_m = n$. The model is:

$$Y_{ij} = \tau_{d(i,j)} + \pi_j + \delta_{d(i,j-1)} + \gamma_i + e_{ij} \qquad (1)$$

where, $i = 1,\ldots,n,$ refers to the unit employed, $j = 1,\ldots,p$ the period, $\tau_{d(ij)} \in \{\tau_{\mathrm{A}}, \tau_{\mathrm{B}}\}$ is the direct effect of the treatment applied, under design d, in the jth period on the ith unit, $\delta_{d(i,j-1)} \in \{\delta_{\mathrm{A}}, \delta_{\mathrm{B}}\}$ is the residual effect of the treatment applied the (j-1)th period on the ith unit, π_j is the jth period effect and γ_i is the ith unit effect. The errors e_{ij} are independent within each unit and among units and have 0 mean and constant variance.

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So the information functions are concave and increasing. Here $nnd(k)$ is for non negative definite $k \times k$ matrix, perm(k) is for permutation $k \times k$ matrix.

Definition 2: A design d^* with information matrix $\mathbf{C}_d^*$ is universally optimal, in the class F of designs, if it maximizes $\varphi(\mathbf{C}_d),\ d \in F$, for all information functions φ .

Definition 3: A design d^* with information matrix $\mathbf{C}_d^*$ is Φ-optimal, in the class F of designs, if $\sum_{i=1}^{v} \varphi\left(\lambda_i\right) \leq \sum_{i=1}^{v} \varphi\left(\mu_i\right)$ for all continuous, decreasing convex functions φ, where $\lambda = (\lambda_1, ..., \lambda_v)$ are the latent roots of $\mathbf{C}_d^*$ and $\mu = (\mu_1, ..., \mu_v)$ are the latent roots of $C_d \ \ \forall\ \ d \in F$.

This is equivalent to: $\lambda \prec \mu$, that is, the vector λ is majorized by the vector μ (Marshall and Olkin p.10).

If a design is universally optimal it is also Φ-optimal and if a design is Φ-optimal, it is A-, D-, E-optimal. Also a design may be optimal for a criterion but not optimal for the other criteria. Note that MV-optimality is not covered by Φ-optimality, since it cannot be expressed as a function of the latent roots of the information matrix.

The idea is to use the concept of majorization in order to establish Φ optimality.

3 Fields of Applications

They will be present in three fields of application of the concept of majorization, one for each different case of experimental designs.

1) The first idea is for Repeated measurements of p periods, two treatments, 2^p sequences (we use the symbolism $s_i\ \ i = 0,1,...,m,$ where $m = 2^p - 1$).

For the estimation of the parameters we have:

If n is the total number of experimental units and $u_i\ \ i = 0,1,...,m$ is the number of experimental units that the sequence s_i of treatments is applied, then $u_0 + u_1 + ... + u_m = n$. The model is:

$$Y_{ij} = \tau_{d(i,j)} + \pi_j + \delta_{d(i,j-1)} + \gamma_i + e_{ij} \tag{1}$$

where, $i = 1, \ldots, n,$ refers to the unit employed, $j = 1, \ldots, p$ the period, $\tau_{d(ij)} \in \{\tau_{\mathrm{A}}, \tau_{\mathrm{B}}\}$ is the direct effect of the treatment applied, under design d, in the jth period on the ith unit, $\delta_{d(i,j-1)} \in \{\delta_{\mathrm{A}}, \delta_{\mathrm{B}}\}$ is the residual effect of the treatment applied the (j-1)th period on the ith unit, π_j is the jth period effect and γ_i is the ith unit effect. The errors e_{ij} are independent within each unit and among units and have 0 mean and constant variance.

The model (1) in vector form is written:

$$\mathbf{Y} = \tau_A \tau_A + \tau_B \tau_B + \delta_A \delta_A + \delta_B \delta_B + \pi_1 \pi_1 + \cdots + \pi_p \pi_p + \gamma_1 \gamma_1 + \cdots \gamma_n \gamma_n + e$$

where $\mathbf{Y}, \tau_A, \tau_B, \delta_A, \delta_B, \pi_1, ..., \pi_p, \gamma_1, ..., \gamma_n, e$ are pn vectors, and $\tau_A\ (\tau_B)$ has 1 when treatment A(B) is applied and 0 elsewhere, that is $\tau_A + \tau_B = 1_{pn}$, $\delta_A(\delta_B)$ has 0 in the first period, 1 when treatment A(B) was applied in the previous period and 0 elsewhere, π_i has 1 in the ith period and 0 elsewhere, thus $\delta_A + \delta_B + \pi_1 = 1_{pn}$, $\pi_1 + \cdots \pi_p = 1_{pn}$. Also $\gamma_i, i = 1, ..., n$ has 1 when the ith unit is employed and 0 e1sewhere, that is, $\gamma_1 + \cdots + \gamma_n = 1_{pn}$.

For the estimation of the parameters of interest not all the other parameters are used (Kounias and Chalikias 2008b). By using the idea of majorization in least squares method, Chalikias and Kounias (2012) have given necessary conditions for Φ-optimality for estimating treatment and residual effects and improved conditions given by Cheng and Wu (1980). This work can be extended to three and more treatments.

2) Another idea is at the Optimal Designs with three treatments in row-column and in factorial designs

The experimental units are arranged in row, there are v treatments and to every unit one of the v treatments is applied. The population is homogeneous with dependent observations. The model in vector form is $y = \mu_1 x_1 + \cdots + \mu_v x_v + e,\ \ E(ee') = \sigma^2 v$, where the $n \times 1$ vector $x_j = (x_{1j}, ..., x_{nj})'$ has $x_{ij} = 1$ when the jth treatment is applied to the ith unit and 0 elsewhere. The errors follow a first order autoregressive AR(1) scheme: $e_i - ae_{i-1} = w_i,\ i = 1, 2, ..., n,\ |a| < 1$, and w_i are uncorrelated random variables with $E(w_i) = 0,\ E(w_i^2) = \sigma^2$. So we have $\mathrm{cov}(e_i, e_j) = \sigma^2 a^{|i-j|} / (1 - a^2)$ and the inverse of the $n \times n$ covariance matrix has the form:

$$\mathbf{V}^{-1} = \mathbf{I_n} + a^2 \begin{bmatrix} 0 & \cdots & 0 \\ \vdots & \mathbf{I_{n-2}} & \vdots \\ 0 & \cdots & 0 \end{bmatrix} - a \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & \ddots & \ddots & 0 \\ 0 & \ddots & \ddots & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}.$$

The parameters of interest are $\mu_1, ..., \mu_v$. The information matrix $\mathbf{Q}$ is: $\mathbf{Q} = \mathbf{X}'\mathbf{V}^{-1}\mathbf{X}, \quad \mathbf{X} = (\mathbf{x}_1, ..., \mathbf{x}_v)$, so

$$\mathbf{Q} = \begin{bmatrix} n_1 & 0 & \cdots & 0 \\ 0 & n_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & n_v \end{bmatrix} + a^2 \begin{bmatrix} \tilde{n}_1 & 0 & \cdots & 0 \\ 0 & \tilde{n}_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \tilde{n}_v \end{bmatrix} - a \begin{bmatrix} 2n_{11} & n_{12} + n_{21} & \cdots & n_{1v} + n_{v1} \\ n_{21} + n_{12} & 2n_{22} & \ddots & \vdots \\ \vdots & \ddots & \ddots & n_{v-1,v} + n_{v,v-1} \\ n_{v1} + n_{1v} & \cdots & n_{v.v-1} + n_{v-1,v} & 2n_{vv} \end{bmatrix}.$$

where,

$n_i \quad i = 1, ..., v$ is the number of times treatment T_i is applied to the n units 1, 2,…,n.

$\tilde{n}_i \quad i = 1, ..., v$ is the number of times treatment T_i appears in the n-2 inside units 2,3,…,n-1.

$n_{ii} \quad i = 1, ..., v$ is the number of times the pair $T_i T_i$ appears in the positions 12,23,…, (n-1)n.

$n_{ij} \quad i \neq j \quad i, j = 1, ..., v$ is the number of times the pair $T_i T_j$ appears in the positions 12,23,…, (n-1)n.

Then applying the averaging rule (Kiefer, 1975) and using the concept of majorization can be found some general rules for the case where the value of a is negative and the case where the value of a is positive. It seems that when a is negative it is easier to handle.

It is proved that: (i) When $0 < a < 1$ in the universally optimal design at most one treatment has a run with length $n_{ii} > 0$. (ii) If $-1 < a < 0$ in the optimal design every pair of distinct treatments appear at most once.

In the case of two treatments S,T and n even: (i) If $0 < a < 1$ the universally optimal design is STST…ST (ii) If $-1 < a < 0$ the universally optimal design is SS..STT…T with S and T in equal numbers.

The model (1) in vector form is written:

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For n odd and two treatments the results are not so simple (i) $0 < a < 1$ the competing designs for optimality are SSTSTS…TST and STST…STS. (ii) $-1 < a < 0$ the competing designs for optimality are SS…STT…T and SS…STT…TS where the numbers of the two treatments differ by 1.

The case of three treatments is more complicated and applying majorization optimal designs under dependence can be found. Also the study can be extended to non homogeneous populations by one or two characteristics, when the number of treatments is three.

3) Another problem is to find optimal designs for 3^k fractional factorial designs for estimating linear and quadratic contrasts.

The problem of finding optimal designs under different types of criteria preoccupied many researchers in the last decades. Most of them dealt with 2^m fractional factorial designs and some cases of general asymmetrical $m_1 \times m_2 \times \ldots \times m_k$ factorials.

Using majorization, as applied to optimal designs Pukelsheim (1993 p.139-142, 352-358) another approach can be used and optimal designs, for estimating linear and quadratic contrasts, for any value of *N*. For this the concept of Balanced Arrays B(*N*,*k*) and Orthogonal Balanced Arrays OBA(*N*,*k*), is introduced, that is, $N \times k$ arrays with three symbols 0, 1, 2, where *N* is the number of runs and *k* is the number of factors involved. The parameters of the OBA(*N*,*k*) will be specified and optimal designs will be given for all values *N*.

Moreover, a demanding problem is to find the maximum number *k* of factors that we can accommodate. An upper bound for the maximum number of factors is (*N*-1)/2. This bound is not attained in most of the cases.

4 Conclusions

The concept of majorization can be a useful tool for designing experiment. Majorization concept can be used to prove Φ-optimality and usually is the only way to do that. As we have seen there are many fields in which majorization can be used and the usage of the method in more fields of experimental design is of interest.

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