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Some applications of weighing designs

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SUMMARY

The purpose of this paper is to apply results on weighing designs to the setting of 2^m factorial designs. Using weighing designs, we give some proposals for experimental plans. Relevant counterexamples are indicated. Also the results of a simulation study on the existence of weighing designs are presented.

Key words: chemical balance weighing design, factorial design, spring balance weighing design

1. Introduction

Let us consider an experiment in which we determine unknown measurements (weights) of given number p objects in n weighing operations. There are two types of weighing designs.

If the objects are distributed over two pans, i.e. they are weighed on a chemical balance, we shall call the corresponding design a two-pan design or chemical balance weighing design. In two-pan weighing the balancing weight may occur on either of the two pans. Let us denote the observation from the i th weighing by y_i, i= 1, 2,…, n, and the weight of the j th object by w_j, j= 1, 2,…, p. The model for estimation of the weights for i= 1, 2,…, n is

$$\mathrm{E}(y_i) = \sum_{i=1}^{p} x_{ij} w_j \,,\ \mathrm{Var}(y_i) = \sigma^2 \,,\ \mathrm{Cov}(y_i, y_{i'}) = 0 \,, \quad (1)$$

where $i \neq i'$, and x_{ij} takes the values +1, -1 or 0 according as the j th object is placed on the left pan, right pan or does not occur in the i th weighing.

If the objects are distributed over one pan of the spring balance, then each observation is a measure of the total weight of the objects placed on the balance pan, and we shall call the corresponding design a one-pan design or spring balance weighing design. Thus in the model for estimation of the weights (1), x_{ij} takes the values 1 or 0, according as the j th object is placed on the pan or does not occur in the i th weighing. In the case of the weighing design, the matrix of the experimental plan (i.e. the matrix that describes in which combinations we put the objects on the pan (pans) of the balance) is the same as the design matrix of the model.

Using matrix notation we can write (1) in the form

$$\mathbf{y} = \mathbf{X}\mathbf{w} + \mathbf{e}, \tag{2}$$

where $\mathbf{X} = (x_{ij})$ is the $n \times p$ design matrix, $\mathbf{w} = (w_1, w_2, ..., w_p)'$ is the vector of unknown measurements of objects, $\mathbf{e}$ is an $n \times 1$ random vector such that $\mathrm{E}(\mathbf{e}) = \mathbf{0}_n$, $\mathrm{Var}(\mathbf{e}) = \sigma^2 \mathbf{I}_n$, where σ^2 is known, $\mathbf{0}_n$ is the $n \times 1$ vector of zeros, and $\mathbf{I}_n$ is the $n \times n$ identity matrix. If $\mathbf{X} \in \mathbf{\Psi}_{n \times p}\{-1,0,1\}$, where $\mathbf{\Psi}_{n \times p}\{-1,0,1\}$ denotes the class of $n \times p$ matrices with elements equal to -1, 0 or 1, (2) is called the model of a chemical balance weighing design. If $\mathbf{X} \in \mathbf{\Phi}_{n \times p}\{0,1\}$, where $\mathbf{\Phi}_{n \times p}\{0,1\}$ denotes the class of matrices $\mathbf{X} = (x_{ij})$ with n rows and p columns and elements x_{ij} equal to 0 or 1, (2) is called the model of a spring balance weighing design. If $\mathbf{X}$ in the model (2) is of full column rank, then all unknown parameters w_j, $j = 1, 2, \ldots, p$, are estimable and the least squares estimate of $\mathbf{w}$ is given by $\hat{\mathbf{w}} = \mathbf{M}^{-1}\mathbf{X}'\mathbf{y}$ with the covariance matrix $\mathrm{Var}(\hat{\mathbf{w}}) = \sigma^2 \mathbf{M}^{-1}$. $\mathbf{M} = \mathbf{X}'\mathbf{X}$ is usually called the information matrix.

The problem is to determine a best design for a fixed number of observations n and objects p. Then the optimality criteria are functions of $\mathbf{M}^{-1}$. One of the possible optimality criteria here is A-optimality (see Pukelsheim, 1993). The design $\mathbf{X}$ is A-optimal, and denoted as $\mathbf{X}_A$, if in the given class of design matrices $\mathrm{tr}(\mathbf{M}^{-1})$ is minimal, i.e. the average variance of estimators is minimal. Moreover, if $\mathrm{tr}(\mathbf{M}^{-1})$ attains the lower bound, the design is called regular A-optimal and is denoted by $\mathbf{X}_r$. It is worth noting here that every regular A-optimal design is always A-optimal, whereas an A-optimal design may or may not be regular A-optimal.

Many problems related to the properties of chemical balance weighing designs, spring balance weighing designs and some aspects of estimation of parameters can be found in the literature; see Kiefer (1974), Banerjee (1975), Katulska (1989), Sathe and Shenoy (1990), Koukouvinos (1995), Ceranka and Graczyk (2001, 2003), Graczyk (2009, 2011, 2012a, b, c). Some applications of weighing designs have been reported, for instance, in Beckman (1973), Banerjee (1975), Sloane and Harwit (1976), Katulska (1984), Ceranka and Katulska (1987a, b, 1989), Koukouvinos (1997).

Weighing designs with n observations and p objects are closely related to 2^m factorial designs. Several theories of factorial designs are presented in Cheng (1980), Montgomery (1991), and Box *et al.* (2005).

Suppose we have m factors A, B, …, each at only two levels. The levels of the factors may be arbitrarily called “low” and “high”. The statistical model for a 2^m design may include the general mean, m main effects, $\binom{m}{2}$ two-factor interactions, $\binom{m}{3}$ three-factor interactions, etc., and one m-factor interaction. This means that for a 2^m design the complete model would contain 2^m effects. The experiment is determined by the plan. Three different notations are commonly used to record the experimental plan. The first is the "+" and "–" notation, often called geometric notation. The second one uses lowercase letter labels to identify the treatment combinations. The third one utilizes 1 and 0 to denote high and low levels of appropriate factors. It is natural to relate "+" and "–" in factorial designs with the notation of "+" and "–" or $+1$ and -1 in the experimental plan of a chemical balance weighing design. Therefore results on optimal chemical balance weighing designs are applicable. Yang and Speed (2002), Glonek and Solomon (2004), and Banerjee and Mukerjee (2008) considered factorial designs under the above parameterization in the context of cDNA microarray experiments. Moreover, in the paper of Mukerjee and Tang (2012), some relations between the experimental plan of the factorial design having 0,1 entries and the experimental plan of the spring balance weighing design are considered. Furthermore, fractional factorial designs of the type 2^{m-q} are considered in the book by Box *et al.* (2005).

We will use the symbol $\mathbf{X}_d$ to denote the matrix of any experimental plan given in the literature.

2. Application of chemical balance weighing designs

In Gawande and Patkar (1999), a factorial experiment of type 2^{5-1} is considered. In the experiment, by the use of a two-level fractional design, the effects of five factors, namely dextrin, peptone, yeast extract, ammonium dihydrogen orthophosphate and magnesium sulfate concentrations, on GCTase production were studied. The experimental plan given in Table III (Gawande and Patkar, 1999), is denoted by means of the symbols "+" and "–". As mentioned above, we relate "+" and "–" in the plan of factorial designs to $+1$ and -1 in the experimental plan of chemical balance weighing designs. So we have

$$\mathbf{X}_d^{'} = \begin{bmatrix} -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\ -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\ -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 \end{bmatrix}. \quad (3)$$

Because of the properties of weighing designs, the matrix of experimental plan $\mathbf{X}_d$ in (3) is the design matrix of the model of a chemical balance weighing design that belongs to the class $\mathbf{\Psi}_{16\times5}\{-1,0,1\}$. We have $\mathbf{X}_d^{'}\mathbf{X}_d = 16\,\mathbf{I}_5$ and $\mathrm{tr}(\mathbf{X}_d^{'}\mathbf{X}_d)^{-1} = 0.3125$. From Ceranka and Katulska (2001), $\mathbf{X}_d$ is the matrix of a regular A-optimal design.

3. Application of spring balance weighing designs

In this section some considerations concerning the experiment described in Seta *et al.* (2000) are addressed.

All of the conclusions presented here are based on experimental data on "Kana" winter oilseed rape growing in the years 1998–1999, as given in Seta *et al.* (2000), table on page 906. In Table 1, we present the part of the data concerning yields in 1999.

The aim of the experiments is to compare the effectiveness of the insecticide Nurelle D 550 EC and four fertilizers adhering to leaves: Basfoliar 12-4-6, Basfoliar 34, Insol B and Solubor DF. The evaluation of the effectiveness of the insecticide and fertilizers was based on the mean number of beetles on a single plant before application and a given number of days after application.

Table 1. The influence of insecticide-fertilizer application on pollen beetle control and yield of winter oilseed rape in 1999

Year 1999		
Treatments	Dose (kg/ha)	Yield (dt/ha)
Nurelle D 550 EC	0.6	2.91
Nurelle D 550 EC + Basfoliar 12-4-6	0.6 + 10.0	2.96
Nurelle D 550 EC + Basfoliar 34	0.6 + 10.0	2.90
Nurelle D 550 EC + Insol B	0.6 + 3.0	3.09
Nurelle D 550 EC + Solubor DF	0.6 + 2.0	3.31

From the description of the experiment we are able to conclude that the experimental plan can be written in the form

$$\mathbf{X}_d = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \end{bmatrix}. \tag{4}$$

We write $\mathbf{w} = (w_1, w_2, \ldots, w_5)'$, where w_1 describes the influence of Nurelle D 550 EC, w_2 describes the influence of Basfoliar 12-4-6, w_3 of Basfoliar 34, w_4 of Insol B and w_5 of Solubor DF. Moreover, $\mathbf{y} = (2.91,\ 2.96,\ 2.9,\ 3.09,\ 3.31)'$, $\mathbf{E(y)} = \mathbf{X}_d\mathbf{w}$. $\mathbf{X}_d$ in (4) is nonsingular, so the w_1, w_2,…, w_5 are estimable and $\hat{\mathbf{w}} = \mathbf{M}_d^{-1}\mathbf{X}_d'\mathbf{y}$, $\mathrm{Var}(\hat{\mathbf{w}}) = \sigma^2\mathbf{M}_d^{-1}$.

The matrix of the experimental plan determines the design matrix of the model. Next, it is expected to be possible to estimate the unknown measurements with small average variance. Thus, one of the possible optimality criteria is A-optimality. For $\mathbf{X}_d$ in the form (4), we obtain $\mathrm{tr}(\mathbf{M}_d^{-1}) = 9$.

In accordance with the notation used in weighing experiments, the experimental plan given by Seta *et al.* (2000), under the assumption that all interactions are equal to zero, can be treated as a spring balance weighing design for estimation of $\mathbf{w} = (w_1, w_2, ..., w_5)'$. Determining the influence of insecticide and four fertilizers in five measurements with the smallest sum of the variances of estimators $\hat{w}_1$, $\hat{w}_2, \ldots,$ $\hat{w}_5$ is equivalent to finding an A-optimal design in the class $\mathbf{\Phi}_{5\times 5}\{0,1\}$. Hence we regard the matrix determining the experiments as the matrix of the experimental plan of a spring balance weighing design, and we suggest taking it in the form

$$\mathbf{X}_s^1 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{bmatrix}. \tag{5}$$

From the above theory, $\hat{\mathbf{w}} = (\mathbf{M}_s^1)^{-1}\mathbf{X}_s^{1'}\,\mathbf{y}$ and $\mathrm{Var}(\hat{\mathbf{w}}) = \sigma^2(\mathbf{M}_s^1)^{-1}$. We obtain $\mathrm{tr}(\mathbf{M}_s^1)^{-1} = 4.(5)$. Hence the sum of variances of the estimators is nearly 2 times smaller than that given in Seta *et al.* (2000) one. Thus it is obvious that if we take the measurements in some combinations, the sum of variances of estimators will be smaller.

If we want significantly to reduce the sum of variances of estimators, then we have to take a greater number of measurements. For this purpose, let us consider the spring balance weighing design for $h = 1$ given by Graczyk (2012c). We take $g = 1$. It is therefore of interest to look at Theorem 3.2(a) for $t = 2$. If $\mathbf{N}$ is the incidence matrix of a balanced incomplete block design with the parameters $v = 5, b = 10, r = 6, k = \lambda = 3$, then $\mathbf{X}_s^2 = \mathbf{N}'$, $\mathbf{X}_s^2 \in \mathbf{\Phi}_{10\times 5}\{0,1\}$. The choice of experimental plan in this form seems to be the best adapted to our theory. For the weighing design the matrix of the experimental plan is the same as the design matrix in the model, so $\mathbf{X}_s^2 \in \mathbf{\Phi}_{10\times 5}\{0,1\}$ is the design matrix of a regular A-optimal spring balance weighing design and

$$\mathbf{X}_s^{2'} = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \end{bmatrix}. \qquad (6)$$

For (6), we get $\mathrm{tr}(\mathbf{M}_s^2)^{-1} = 1.3(8)$.

Our approach sheds some new light on the adaptation of spring balance weighing designs to such experiments, making it possible to determine the experimental plan giving the design matrix $\mathbf{X}$ with required properties. We are also able to obtain estimators with much smaller average variance.

Now, let us consider the second part of the data given in Seta *et al.* (2000). The results are given in Table 2. In this part of the experiment the influence of the insecticide Bulldock 025 EC and the three fertilizers Basfoliar 36 Extra, Basfoliar 12-4-6 and Basfoliar 34 is determined.

Table 2. The influence of insecticide-fertilizer application on pollen beetle control and yield of winter oilseed rape in 1998

Year 1998		
Treatments	Dose (kh/ha)	Yield (dt/ha)
Bulldock 025 EC	0.25	3.89
Bulldock 025 EC + Basfoliar 36 Extra	0.25 + 10.0	4.26
Bulldock 025 EC + Basfoliar 12-4-6	0.25 + 10.0	4.06
Bulldock 025 EC + Basfoliar 34	0.25 + 10.0	3.43

For convenience and clarity, let us denote by w_1 the influence of Bulldock 025 EC, w_2 the influence of Basfoliar 36 Extra, w_3 the influence of Basfoliar 12-4-6, and w_4 the influence of Basfoliar 34. Similarly as in the theory presented in the first part of this section, from the description of the experiment we can derive that $\mathbf{y} = (3.89,\ 4.26,\ 4.06,\ 3.43)'$, $\mathbf{w} = (w_1, w_2, w_3, w_4)'$. The plan of this experiment has the form:

$$\mathbf{X}_d = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}. \tag{7}$$

Moreover, we have $\mathbf{E}(\mathbf{y}) = \mathbf{X}_d \mathbf{w}$. $\mathbf{X}_d$ in (7) is nonsingular, so w_1, w_2, w_3, w_4 are estimable and $\mathrm{Var}(\hat{\mathbf{w}}) = \sigma^2 (\mathbf{M}_d)^{-1}$.

Under the assumption that all interactions in the experiment given by Seta *et al.* (2000) are zeros, let us consider the theory given in the paper of Graczyk (2011). The important point to note here is the form of the matrix of the experimental plan. In the above experiment, the insecticide occurs in each measurement, therefore we treat it as a bias. Under the above assumption, in this experiment we determine the influence of three factors. From Graczyk (2011), the matrix $\mathbf{X}_d$ in (7) can be written as the matrix of the experimental plan of a spring balance weighing design with bias

$$\mathbf{X}_d = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & \mathbf{x}' \\ \mathbf{1}_3 & \mathbf{X}_d^* \end{bmatrix} = [\mathbf{1}_4 \quad \mathbf{X}_{d1}], \tag{8}$$

where $\mathbf{X}_d^* = \mathbf{I}_3$ and $\mathbf{x} = \mathbf{0}_3$. Now, let us consider formula (7) given by Graczyk (2011). For $\mathbf{X}_d$ in (8), we have $\mathrm{tr}(\mathbf{M}_{d1})^{-1} = 3$. We now apply Theorem 3.4 (ii) for $\mathbf{x} = \mathbf{0}_3$. We obtain

$$\mathbf{X}_s^3 = \begin{bmatrix} 1 & \mathbf{x}' \\ \mathbf{1}_3 & \mathbf{X}_s^* \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix} = [\mathbf{1}_4 \quad \mathbf{X}_{s1}],$$

where $\mathbf{X}_s^* = \mathbf{N}'$, $\mathbf{N}$ is the incidence matrix of the balanced incomplete block design with parameters $v = b = 3,\ r = k = 2,\ \lambda = 1$ in the form

$$\mathbf{N} = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix}.$$

$\mathbf{X}_s^3$ is the experimental plan and simultaneously is the design matrix of a regular A-optimal spring balance weighing design with bias. Further, we have $\mathrm{tr}(\mathbf{M}_{s1})^{-1} = 2.25$. This means that we are able to estimate the influence of the insecticide and three fertilizers with smaller average variance of estimators.

4. Simulation study

In this section we present some problems which arise when determining a regular A-optimal spring balance weighing design. The main difficulty in carrying out this construction is that in any class $\mathbf{\Phi}_{n\times p}(0,1)$ a regular A-optimal design may not exist.

As an example, let us consider an experiment in which we determine unknown measurements of $p = 4$ objects in $n = 5$ measurements. We assume that the measurement errors are uncorrelated and they have the same variances, so the model of the spring balance weighing design is given by (2) and the design matrix $\mathbf{X}$ belongs to the class $\mathbf{\Phi}_{5\times 4}\{0,1\}$. From Graczyk (2012c), Theorem 2.1, we have $\mathrm{tr}(\mathbf{M}^{-1}) \geq 2$. Moreover, Theorem 2.2(a) implies that $\mathbf{X}$ is the matrix of a regular A-optimal spring balance weighing design if and only if $\mathrm{tr}(\mathbf{M}^{-1}) = 2$, and moreover the optimality condition requires $\mathbf{X}'\mathbf{X} = 5(2\mathbf{I}_5 + \mathbf{1}_5\mathbf{1}_5')/6$. Seeing that $\mathbf{X} \in \mathbf{\Phi}_{5\times 4}\{0,1\}$, this optimality condition is not satisfied. So, in the class $\mathbf{\Phi}_{5\times 4}\{0,1\}$ we are not able to determine a matrix $\mathbf{X}$ for which $\mathrm{tr}(\mathbf{M})^{-1} = 2$. Thus in this class a regular A-optimal spring balance weighing design $\mathbf{X}_{r}$ does not exist.

We are interested in determining all unknown measurements of objects, so we have to fix all nonsingular design matrices $\mathbf{X} \in \mathbf{\Phi}_{5\times 4}\{0,1\}$. In order to give the optimal design, for each $\mathbf{X}$, we find $\mathrm{tr}(\mathbf{M})^{-1}$. As the next step we have to show how much $\mathrm{tr}(\mathbf{M})^{-1}$ of any $\mathbf{X} \in \mathbf{\Phi}_{5\times 4}\{0,1\}$ differs from $\mathrm{tr}(\mathbf{M}_{r})^{-1}$.

Let us consider the theory given by Graczyk (2012c) for $s=1$ and $g=1$. According to the notation given in this paper, $\mathbf{G}=\mathbf{I}_5$ and $\mathbf{X}_1=\mathbf{X}$. Similarly as in the proof of Theorem 2.1 we assume that the number of elements equal to 1 in each row of the design matrix $\mathbf{X}$ is constant, i.e. $\mathbf{X}\mathbf{1}_p=k\mathbf{1}_n$. Notice that if the design matrix $\mathbf{X}_\eta$ is constructed from the design matrix $\mathbf{X}_\kappa$ through permutation of its rows (or columns), then the designs $\mathbf{X}_\eta$ and $\mathbf{X}_\kappa$ are the same, because the permutation of rows in $\mathbf{X}_\eta$ is interpreted as a renumbering of objects (or weighings).

The results of a simulation study for determining unknown measurements of $p=4$ objects in $n=5$ measurements are given in Table 3.

Table 3. Traces of the inverse of the information matrix for the design matrix $\mathbf{X}\in\mathbf{\Phi}_{5\times 4}\{0,1\}$

	$\mathrm{tr}(\mathbf{M})^{-1}=2.5$	$\mathrm{tr}(\mathbf{M})^{-1}=2.7(2)$	$\mathrm{tr}(\mathbf{M})^{-1}=3.5$
Percentage of designs	8.1%	5.4%	86.5%

The number of all nonsingular design matrices $\mathbf{X}\in\mathbf{\Phi}_{5\times 4}\{0,1\}$ is 74. To sum up, only 8.1% of matrices $\mathbf{X}$ are matrices of an A-optimal spring balance weighing design $\mathbf{X}_A$, and then $\mathrm{tr}(\mathbf{M}_A)^{-1}-\mathrm{tr}(\mathbf{M}_r)^{-1}=0.5$. Hence $\mathrm{tr}(\mathbf{M}_A)^{-1}$ for the A-optimal spring balance weighing design will have increased by 25% with respect to $\mathrm{tr}(\mathbf{M}_r)^{-1}$ for the regular A-optimal spring balance weighing design $\mathbf{X}_r$. Next, let us consider any other matrix $\mathbf{X}\in\mathbf{\Phi}_{5\times 4}\{0,1\}$. For 5.4% of the design matrices $\mathrm{tr}(\mathbf{M})^{-1}-\mathrm{tr}(\mathbf{M}_r)^{-1}=0.7(2)$, i.e. the sum of variances of estimators will have increased by 36% with respect to $\mathrm{tr}(\mathbf{M}_r)^{-1}$. Moreover, for 86.5% of the design matrices $\mathbf{X}\in\mathbf{\Phi}_{5\times 4}\{0,1\}$, $\mathrm{tr}(\mathbf{M})^{-1}-\mathrm{tr}(\mathbf{M}_r)^{-1}=1.5$, i.e. the sum of variances of estimators will have increased by 75% with respect to the sum for the regular A-optimal design.

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