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ScienceDirect
Journal of Statistical Planning and Inference 138 (2008) 4093–4106
journal of statistical planning and inference
www.elsevier.com/locate/jspi

D-optimal designs for correlated random vectors☆

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Received 28 February 2007; received in revised form 3 March 2008; accepted 7 March 2008
Available online 13 March 2008

Abstract

Suppose that $Y=(Y_i)$ is a normal random vector with mean Xb and covariance $\sigma^2 I_n$, where b is a p-dimensional vector (b_j), $X=(X_{ij})$ is an $n\times p$ matrix. Given a family $\mathscr{D}$ of D-optimal designs, a design Z in $\mathscr{D}$ is chosen that is robust in the sense that Z is D-optimal in $\mathscr{D}$ when the components Y_i are dependent: for $i\neq i'$, the covariance of $Y_i, Y_{i'}$ is $\rho\neq 0$. Such designs Z merely depend on the sign of ρ. The general results are applied to the situation where $X_{ij}\in\{-1,1\}$; this corresponds to a factorial design with -1, 1 representing low or high level, respectively, or corresponds to a weighing design with -1, 1 representing an object j with weight b_j being placed on the left and right side of a chemical balance, respectively.

MSC: primary 62K05; secondary 62H10

Keywords: Chemical balance; Correlation; Determinant; D-optimal design; Factorial design; Hadamard matrix; Randomized effect; Weighted least square estimator

1. Introduction

Let $Y=(Y_i)$ be a normal n-dimensional random vector with mean $\mu=Xb$, where $X=(X_{ij})$ is an $n\times p$ matrix of rank p with each X_{ij} in the set $\Re$ of real numbers, $b=(b_j)$ is a parameter in the p-dimensional Euclidean space $\Re^p$, and the covariance, Σ_Y, of Y is $\sigma^2 I_n$, where $\Re$ denotes the real line. To simplify our presentation, we assume that $\sigma=1$. The precision of the least square estimator $\tilde{b}(Y)$ and of the usual confidence ellipsoid of b depends only on covariance, $\operatorname{cov}(\tilde{b}(Y))$, of $\tilde{b}(Y)$, where

$$\tilde{b}(Y)=(X'X)^{-1}X'Y, \tag{1.1}$$

and

$$\operatorname{cov}(\tilde{b}(Y))=(X'X)^{-1}. \tag{1.2}$$

So we wish to choose an X such that, among all admissible designs X, $(X'X)^{-1}$ is smallest in some way, e.g., to choose X such that X is D-optimal, i.e., the generalized variance

$$|\operatorname{cov}(\tilde{b}(Y))|=|(X'X)^{-1}| \tag{1.3}$$

is smallest, where $|\bullet|$ denotes the determinant function.

☆ Research supported by NSERC Grant of Canada, PIN7914.
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0378-3758/$ - see front matter
doi:10.1016/j.jspi.2008.03.012

Due to random effects or practical circumstance, $\mathrm{cov}(Y_i, Y_{i'}) = \rho$ with ρ positive or negative; see, e.g., Searle (1971) and Pukelsheim (1993). On the other hand, when $\rho = 0$, there may exist more than one D-optimal design X. For example, for the weighing design model, there may be a large family of D-optimal designs (see Galil and Kiefer, 1980). Because of this, one may wish to set up a criterion to choose a particular one; see, e.g., Galil and Kiefer (1983). Consideration of $\rho \neq 0$ is such a criterion. Other authors have addressed similar problems (see Ceranka and Graczyk, 2004; Ceranka et al., 2006; Das et al., 2003; Evangelaras et al., 2002).

Now, the weighted least square estimator $\tilde{b}(Y)$ is given by

$$\tilde{b}(Y) = (X'G^{-1}X)^{-1}X'G^{-1}Y, \tag{1.4}$$

where $G = \Sigma_Y$:

$$G = (1-\rho)I_n + \rho J_n, \quad \frac{-1}{n-1} < \rho < 1, \tag{1.5}$$

$$J_n = e_n e_n', \quad e_n = (1, 1, \ldots, 1)' \in \Re^n. \tag{1.6}$$

Since

$$\mathrm{cov}(\tilde{b}) = (X'G^{-1}X)^{-1}.$$

X is D-optimal with respect to ρ if it minimizes $|(X'G^{-1}X)^{-1}|$, or equivalently, maximizes $|X'G^{-1}X|$.

Although all of our main results in Section 2 are general, we shall merely apply them to the case where $X_{ij} \in \{-1, 1\}$. More specifically, let $\mathscr{D}$ be the set of D-optimal designs obtained earlier for $\rho = 0$, i.e., $X \in \mathscr{D}$ maximizes $|X'X|$ for X in $\mathscr{D}$. We shall choose a design Z in $\mathscr{D}$ such that it is robust in the sense that it also maximizes $|X'G^{-1}X|$ for all $X \in \mathscr{D}$ and all $\rho > 0$ (< 0). This definition of robustness guards against the situation where the experimenter assumes the observations Y_i are uncorrelated when, in fact, there may be a positive (negative) correlation.

The models Y considered here correspond to certain factorial designs with $-1, 1$ representing low or high level, respectively, or correspond to weighing designs with $-1, 1$ representing the object j with weight b_j being placed on the left and right side of a chemical balance, respectively; see, e.g., Cheng (1978, 1980, 1987), Cheng et al. (1985), Galil and Kiefer (1982, 1983), Jacroux et al. (1983), Pukelsheim (1993), Sathe and Shenoy (1991). The results on optimal designs in these papers are subject to the existence of an $m \times m$ Hadamard matrix, $H = (h_{ij})$, of appropriate order m:

$$\text{all } i, j \in \{-1, 1\}, \quad H'H = mI_m. \tag{1.7}$$

The existence of such a matrix is still a conjecture for $m = 268$ and many other $m > 268$; see Hedayat and Wallis (1978). For other D-optimal designs, see, e.g., Chen and Huang (2000), Huang (1987), Huang et al. (1995), Pukelsheim (1993), Yeh and Huang (2005).

2. Main results

We begin by simplifying $\mathrm{cov}(\tilde{b}) = (X'G^{-1}X)^{-1}$. Let $M_{n\times p}$ be the set of all $n \times p$ matrices over $\Re$ equipped with the trace norm $\|\bullet\| : \|A\| = (\mathrm{tr}(A'A))^{1/2}$. Note that $M_{n\times p} = \Re^n$ if $p = 1$. We shall first estimate $\|u(X)\|^2$, where

$$u(X) = (X'X)^{-1/2}X'e_n, \tag{2.1}$$

a very important vector in our presentation (e_n is as in (1.6)).

Lemma 1. *Let $X \in M_{n\times p}$. Then*:

(a)

$$\|u(X)\|^2 \leqslant n. \tag{2.2}$$

(b) *Suppose that $X'X = nI_p$. Then $\|X'e_n\| \leqslant n$. Hence if e_n is a column of X, then $\|X'e_n\| = n$.*