



Computing c -optimal experimental designs using the simplex method of linear programming

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ABSTRACT

An experimental design is said to be c -optimal if it minimizes the variance of the best linear unbiased estimator of $c^T\beta$, where c is a given vector of coefficients, and β is an unknown vector parameter of the model in consideration. For a linear regression model with uncorrelated observations and a finite experimental domain, the problem of approximate c -optimality is equivalent to a specific linear programming problem. The most important consequence of the linear programming characterization is that it is possible to base the calculation of c -optimal designs on well-understood computational methods. In particular, the simplex algorithm of linear programming applied to the problem of c -optimality reduces to an exchange algorithm with different pivot rules corresponding to specific techniques of selecting design points for exchange. The algorithm can also be applied to “difficult” problems with singular c -optimal designs and relatively high dimension of β . Moreover, the algorithm facilitates identification of the set of all the points that can support some c -optimal design. As an example, optimal designs for estimating the individual parameters of the trigonometric regression on a partial circle are computed.

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1. Introduction

Consider the linear regression model $(\mathbf{f}, \mathcal{X})$ with uncorrelated homoscedastic observations y satisfying $E(y) = \mathbf{f}^T(x)\beta$, where β is an unknown m -dimensional parameter and \mathbf{f} is a known vector of regression functions linearly independent on the experimental domain $\mathcal{X} = \{x_1, \dots, x_k\}$. Let \mathbf{c} be a fixed nonzero m -dimensional vector.

The main purpose of this paper is to propose an algorithm based on the simplex method of linear programming for constructing \mathbf{c} -optimal approximate designs for the model $(\mathbf{f}, \mathcal{X})$. An experimental design $\xi_{\mathbf{c}}^*$ is said to be \mathbf{c} -optimal if, under $\xi_{\mathbf{c}}^*$, the best linear unbiased estimator of $\mathbf{c}^T\beta$ has the minimal possible variance (see (2) for a more precise definition). For instance, if \mathbf{c} is the i -th unit vector $\mathbf{e}_i \in \mathbb{R}^m$, then $\xi_{\mathbf{c}}^*$ is optimal for estimating individual parameters β_i , if $\mathbf{c} = \mathbf{f}(x)$, then $\xi_{\mathbf{c}}^*$ is optimal for estimating the mean value of response in x , and so on. Moreover, \mathbf{c} -optimal designs are closely related to several other criteria of design optimality, in particular the so-called standardized criteria (see Dette (1997)). We refer the reader to Pázman (1986) and Pukelsheim (1993) for details on general optimal design of experiments.

As is usual, by an approximate design we understand a probability ξ on \mathcal{X} with the interpretation that $\xi(x)$ represents the proportion of the measurements to be taken in x . The set of all approximate designs on \mathcal{X} will be denoted by \mathcal{E} . A design $\xi \in \mathcal{E}$ is said to be an exact design of size n , if and only if (iff) it can be realized by n measurements, i.e., iff $\xi(x_j) = n_j/n$ for all $j = 1, \dots, k$ and some $n_j \in \mathbb{N} \cup \{0\}$.

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Let \mathcal{E}_c be the set of all the designs $\xi \in \mathcal{E}$ that guarantee estimability of $\mathbf{c}^T \beta$, i.e., such that \mathbf{c} belongs to the range of the information matrix

$$\mathbf{M}(\xi) = \sum_{x \in \mathcal{X}} \mathbf{f}(x) \mathbf{f}^T(x) \xi(x). \tag{1}$$

If we perform n measurements according to an exact design $\xi \in \mathcal{E}_c$ of size n , and if $\hat{\beta}_\xi$ is the least squares estimate of β , then the variance of the best linear unbiased estimator of the linear combination $\mathbf{c}^T \beta$ is

$$\text{Var}(\mathbf{c}^T \hat{\beta}_\xi) = \sigma^2 n^{-1} \mathbf{c}^T \mathbf{M}^{-}(\xi) \mathbf{c}, \tag{2}$$

where σ^2 is the variance of the individual observations y , and $\mathbf{M}^{-}(\xi)$ is a pseudoinverse of $\mathbf{M}(\xi)$. Note that for $\xi \in \mathcal{E}_c$ the value $\mathbf{c}^T \mathbf{M}^{-}(\xi) \mathbf{c}$ does not depend on the choice of the pseudoinverse.

Equality (2) motivates the following definition: Any design $\xi_c^* \in \mathcal{E}_c$ that minimizes $\mathbf{c}^T \mathbf{M}^{-}(\xi) \mathbf{c}$ among all designs $\xi \in \mathcal{E}_c$ is said to be \mathbf{c} -optimal for the model $(\mathbf{f}, \mathcal{X})$. We define the \mathbf{c} -optimal variance of the model $(\mathbf{f}, \mathcal{X})$ to be $\mathbf{c}^T \mathbf{M}^{-}(\xi_c^*) \mathbf{c}$, and the \mathbf{c} -optimal information matrix to be the information matrix of any \mathbf{c} -optimal design. It is possible to show that a \mathbf{c} -optimal design always exists, but it does not have to be unique. Moreover, for many standard models and choices of the vector \mathbf{c} , some or all of the \mathbf{c} -optimal information matrices are singular.

The Elfving set of the model $(\mathbf{f}, \mathcal{X})$ is defined by

$$\mathcal{E} = \text{conv}(\mathbf{f}(\mathcal{X}) \cup -\mathbf{f}(\mathcal{X})),$$

where $\mathbf{f}(\mathcal{X}) = \{\mathbf{f}(x_1), \dots, \mathbf{f}(x_k)\}$ and conv is the convex hull. By $\partial \mathcal{E}$ we will denote the boundary of \mathcal{E} . The Elfving theorem can be formulated as follows (Elfving (1952); see also Pázman (1986) or Pukelsheim (1993)).

Theorem 1. *Let $\xi \in \mathcal{E}$. Then the following statements are equivalent:*

- (i) *The design ξ is \mathbf{c} -optimal for $(\mathbf{f}, \mathcal{X})$;*
- (ii) *There exists $h > 0$ and a selection of signs $\epsilon(x) \in \{-1, 1\}$ for all $x \in \mathcal{X}$, such that*

$$h \mathbf{c} = \sum_{x \in \mathcal{X}} \epsilon(x) \mathbf{f}(x) \xi(x) \in \partial \mathcal{E}. \tag{3}$$

In such a case h^{-2} is the \mathbf{c} -optimal variance of the model $(\mathbf{f}, \mathcal{X})$.

In López-Fidalgo and Rodríguez-Díaz (2004), the Elfving theorem has been used to construct algorithms for \mathbf{c} -optimal designs (with a compact experimental domain, possibly infinite) requiring constrained nonlinear optimization routines and achieving a practically efficient performance for dimensions m up to 4. In the present paper, we use the Elfving theorem to reformulate the problem of constructing a \mathbf{c} -optimal design on a finite experimental domain as a specific problem of linear programming (LP). As a consequence, questions regarding \mathbf{c} -optimality on a finite experimental domain can be directly answered by the extensive theory of LP. Moreover, LP gives us algorithmic tools for calculating \mathbf{c} -optimal designs (such as the simplex method) that are rapid and reliable even in the case of relatively high dimensions of the parameter. With present computer hardware, the algorithm can be applied to problems with a very large experimental domain (e.g. thousands of design points). Thus, even in the case of an infinite experimental domain such as an interval, it is often possible to use a dense discretization with a negligible loss of efficiency.

2. Linear programming characterization of \mathbf{c} -optimal designs

By the Elfving theorem, constructing a \mathbf{c} -optimal design is equivalent to finding the maximum scalar h , such that the vector $h \mathbf{c}$ belongs to the Elfving set. For the finite experimental domain \mathcal{X} , the Elfving set is a polytope, hence the \mathbf{c} -optimal design problem is equivalent to the specific problem of LP formulated below in Theorem 2. Our reference monographs for LP are Dantzig and Thapa (1997) and Vanderbei (2001). For simplicity, let $\mathbf{F} = (\mathbf{f}_1, \dots, \mathbf{f}_{2k})$, where

$$\mathbf{f}_j = \begin{cases} \mathbf{f}(x_j), & j \in \{1, \dots, k\} \\ -\mathbf{f}(x_{j-k}), & j \in \{k+1, \dots, 2k\}. \end{cases} \tag{4}$$

Theorem 2. *Let $\xi \in \mathcal{E}$. Then the following statements are equivalent:*

- (i) *The design ξ is \mathbf{c} -optimal for $(\mathbf{f}, \mathcal{X})$ and h^{-2} is the \mathbf{c} -optimal variance of the model $(\mathbf{f}, \mathcal{X})$;*
- (ii) *$\xi(x_j) = \alpha_j + \alpha_{j+k}$ for all $j = 1, \dots, k$ and for some solution $(\alpha^T, h)^T \in \mathbb{R}^{2k+1}$ of the LP problem:*

$$\max \left\{ h \mid \begin{pmatrix} \mathbf{F} & -\mathbf{c} \\ \mathbf{1}_{2k}^T & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ h \end{pmatrix} = \begin{pmatrix} \mathbf{0}_m \\ 1 \end{pmatrix}, \alpha \geq \mathbf{0}_{2k}, h \geq 0 \right\}. \tag{5}$$

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