GEOMETRY OF E-OPTIMALITY

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Holger Dette
Inst. für Math. Stochastik
Universität Göttingen
Lotzestr. 13
3400 Göttingen, GERMANY

and

William J. Studden
Department of Statistics
Purdue University
1399 Mathematical Sciences Bldg
West Lafayette, IN 47907-1399

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Holger Dette
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Universität Göttingen
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William J. Studden
Department of Statistics
Purdue University
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West Lafayette, IN 47907-1399, USA

Abstract

In the usual linear model $y = \theta' f(x)$ we consider the E-optimal design problem. A sequence of generalized Elfving sets $\mathcal{R}_k \subseteq \mathbb{R}^{n \times k}$ (where n is the number of regression functions) is introduced and the corresponding inball radii are investigated. It is shown that the E-optimal design is an optimal design for $A'\theta$ where $A \in \mathbb{R}^{n \times n}$ is any inball vector of a generalized Elfving set $\mathcal{R}_n \subseteq \mathbb{R}^{n \times n}$. The minimum eigenvalue of the E-optimal design can be identified as the corresponding squared inball radius of $\mathcal{R}_n$. A necessary condition for the support points of the E-optimal design is given by a consideration of the supporting hyperplanes corresponding to the inball vectors of $\mathcal{R}_n$.

The results presented allow the determination of E-optimal designs by an investigation of the geometric properties of a convex symmetric subset $\mathcal{R}_n$ of $\mathbb{R}^{n \times n}$ without using any equivalence theorems. The application is demonstrated in several examples solving elementary geometric problems for the determination of the E-optimal design. In particular we give a new proof of the E-optimal spring balance and chemical balance weighing (approximate) designs.

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1. Introduction. Let $f(x) = (f_1(x), \ldots, f_n(x))'$ denote n linearly independent regression functions on a compact set $\mathcal{X}$ which contains at least n points and let $\theta = (\theta_1, \ldots, \theta_n)'$ denote a vector of parameters. We will consider the usual linear regression model in which for every $x \in \mathcal{X}$ a random variable $Y(x)$ with mean $\theta' f(x)$ and variance $\sigma^2 > 0$ can be observed. An experimental design is a probability measure ξ defined on a σ-field of sets of $\mathcal{X}$ which include the one point sets. The information matrix of the design ξ is given by

$$M(\xi) = \int_{\mathcal{X}} f(x) f'(x) d\xi(x).$$

If ξ concentrates mass n_i/N at the points x_i $(i = 1, \ldots, r, \sum_{j=1}^{r} n_i = N)$ the experimenter takes n_i uncorrelated observations at each x_i $(i = 1, \ldots, r)$ and the covariance matrix of the least squares estimator for θ is proportional to $M^{-1}(\xi)$. An optimal design maximizes or minimizes an appropriate functional of the information matrix or its inverse. In this paper we will investigate the E-optimality criterion which maximizes the minimum eigenvalue of $M(\xi)$ with respect to the design ξ. The E-optimal design minimizes the worst possible variance of the least squares estimators for all possible linear combinations $c'\theta$ where $c \in \mathbb{R}^n$ has euclidean norm 1. For this reason the E-optimal design problem is intimately related to the problem of optimal design for linear combinations of the unknown parameter vector which is considered next.

Let $k \leq n$ and $A \in \mathbb{R}^{n \times k}$ denote a real valued matrix. A design ξ is called optimal for $A'\theta$ if it minimizes $tr(M^-(\xi)AA')$ where $M^-(\xi)$ denotes a generalized inverse of $M(\xi)$ and $tr(B)$ the trace of a matrix B. An optimal design for $A'\theta$ can be used if the experimenter is interested in certain linear combinations $a_1'\theta, \ldots, a_k'\theta$ of the unknown parameter vector where $a_1, \ldots, a_k$ denote the columns of the matrix A.

If the minimum eigenvalue of the E-optimal moment matrix has multiplicity one there is a nice geometric interpretation of the minimum eigenvalue $\lambda_{\min}$ and its corresponding normalized eigenvector a_1 $(||a_1||_2 = 1)$ (see Pukelsheim and Studden (1991)). In this case the design ξ is E-optimal if and only if it is optimal for $a_1'\theta$. Moreover, the vector $\sqrt{\lambda_{\min}}\, a_1$ is an inball vector of the Elfving set

$$\mathcal{R}_1 = \text{ conv } (\{\varepsilon f(x) | x \in \mathcal{X}, \varepsilon = \mp 1\}) \subseteq \mathbb{R}^n, \tag{1.1}$$

where conv (S) denotes the convex hull of S. This means that the ball $\{x| \; ||x||_2^2 \leq \lambda_{\min}\}$ is the largest ball which is included in the set $\mathcal{R}_1$ (here $||\cdot||_2$ denotes the euclidean norm on

$\mathbb{R}^n$) and the vector $\sqrt{\lambda_{\min}}a_1$ is on the boundary of $\mathcal{R}_1$. The set $\mathcal{R}_1$ is due to Elfving (1952) and is very useful in discussing optimal designs for $c'\theta$ where $c \in \mathbb{R}^n$ (see also Pukelsheim (1981) or Studden (1971)). The above result suggests the following procedure for finding E-optimal designs. At first the inball radius r_1 and a corresponding inball vector a_1 are determined and then using the results on scalar-optimality the optimal design for $a_1'\theta$ is found. Under the assumption that the minimum eigenvalue of the E-optimal design has multiplicity 1 the resulting design is the E-optimal one. An obvious drawback of this procedure is that the multiplicity of the minimum eigenvalue is unknown because the E-optimal design (which has to be determined by it) is not known. A simple striking example in which E-optimality is obtained without any scalar optimality was given by Pukelsheim (1981), Example 5.

It is the purpose of this paper to develop a characterization of E-optimality without any assumption on the multiplicity of the minimum eigenvalue of the E-optimal design. After stating some preliminary results from the literature in section 2 we will show in section 3 that every E-optimal design is optimal for a set of parameters $A'\theta$ where the matrix A essentially contains some of the eigenvectors corresponding to the minimum eigenvalue of the E-optimal moment matrix. We will introduce generalized Elfving sets $\mathcal{R}_k$ and give a similar geometric characterization of the minimum eigenvalue of the E-optimal design (with an arbitrary multiplicity) as an inball radius of one of these sets. This result provides a procedure for the geometric determination of E-optimal designs without any prior knowledge of the multiplicity of the minimum eigenvalue. The application of the results is illustrated by several examples in section 4. In particular we present an elementary (geometric) derivation of the E-optimal spring balance weighing designs which were considered (among other things) by Cheng (1987).

2. Preliminaries. In this section we will discuss some important tools used in determining E-optimal designs and optimal designs for $A'\theta$ where $A \in \mathbb{R}^{n\times k}$ is a given matrix. The following two equivalence theorems enjoy particular popularity and can be found in Pukelsheim (1980).

Theorem 2.1 (E-optimality). A design ξ_E is E-optimal (i.e. it maximizes the minimum eigenvalue of $M(\xi)$) if and only if there exists a matrix $E \in$ conv (S) such that

$$f'(x)Ef(x) \leq \lambda_{\min} \text{ for all } x \in \mathcal{X}. \tag{2.1}$$

Here $\lambda_{\min}$ denotes the minimum eigenvalue of the matrix $M(\xi_E) \in \mathbb{R}^{n\times n}$ and conv (S) is the convex hull of the set S of all $n \times n$ matrices of the form zz', with $||z||_2 = 1$, such that z is an eigenvector of $M(\xi_E)$ corresponding to $\lambda_{\min}$.

Theorem 2.2 (Optimality for $A'\theta$). Let $A \in \mathbb{R}^{n\times k}$ denote a given matrix of rank k and ξ_A denote a design for which range $(A) \subseteq$ range $(M(\xi_A))$. The design ξ_A is optimal for $A'\theta$ if and only if there exists a generalized inverse G of $M(\xi_A)$ such that

$$tr(A'Gf(x)f'(x)G'A) \leq tr(A'M^{-}(\xi_A)A) \text{ for all } x \in \mathcal{X}.$$

The following theorem was proved by Studden (1971) and is a generalization of the famous theorem of Elfving (1952) for scalar optimality. If provides a geometric characterization of the optimal design for $A'\theta$ by considering boundary points of a symmetric convex subset of $\mathbb{R}^{n\times k}$. Define

$$\mathcal{R}_k = \text{ conv } (\{f(x)\varepsilon' | x \in \mathcal{X}, \varepsilon \in \mathbb{R}^k, ||\varepsilon||_2 = 1\}) \subseteq \mathbb{R}^{n\times k}, \tag{2.2}$$

(note that this definition corresponds to (1.1) for $k = 1$); we have the following result.

Theorem 2.3 (Elfving's Theorem for $A'\theta$). A design $\xi = \left\{ \begin{smallmatrix} x_i \\ p_i \end{smallmatrix} \right\}_{i=1}^{m}$ is optimal for $A'\theta$ if and only if there exists a number $\gamma > 0$ and vectors $\varepsilon_1, \ldots, \varepsilon_m \in \mathbb{R}^k$ with euclidean norm 1 such that the point

$$\gamma A = \sum_{i=1}^{m} p_i f(x_i)\varepsilon_i' \tag{2.3}$$

is a boundary point of the set $\mathcal{R}_k$.

For the application of this result we will need an appropriate characterization of the boundary points of $\mathcal{R}_k$. For convex subsets of $\mathbb{R}^n$ boundary points can be characterized by supporting hyperplanes. The same is still true for (convex) subsets of $\mathbb{R}^{n\times k}$ when the vectors are replaced by matrices. More precisely we have the following result (see Studden (1971), Lemma 3.2).

Lemma 2.4. A matrix γA of the form (2.3) is a boundary point of $\mathcal{R}_k$ if and only if there exists a "supporting hyperplane" $D \in \mathbb{R}^{n\times k}$ such that

(i) $tr(\gamma A'D) = 1$

(ii) $||D'f(x)||_2^2 = f'(x)DD'f(x) \leq 1$ for all $x \in \mathcal{X}$

and equality holds in (ii) for each x_i with $p_i > 0$. Moreover we have $\varepsilon_i = D'f(x_i)$ $(i = 1, \ldots, m)$ in the representation (2.3).

For our later investigations it is useful to identify the supporting hyperplane of the boundary point γA in (2.1) of Theorem 2.3. It follows from the proof of this theorem (see Studden (1971)) that

$$\gamma A = M(\xi_A)D \tag{2.4}$$

where $M(\xi_A)$ is the information matrix of the optimal design for $A'\theta$. Moreover we have for the number γ in this theorem

$$\gamma^{-2} = tr(A'M^{-}(\xi_A)A) \tag{2.5}$$

for any generalized inverse of $M(\xi_A)$ and for the supporting hyperplane D we obtain

$$trD'M(\xi_A)D = 1.$$

3. Main results. In this section we will investigate the relationship between the E-optimal design and the optimal designs for $A'\theta$. In what follows $\lambda_{\min}$ always denote the minimum eigenvalue of the information matrix of the E-optimal design ξ_E and $\lambda_{\min}(B)$ denotes the minimum eigenvalue of a matrix B. By Theorem 2.1 the design ξ_E is E-optimal if and only if there exists a matrix E which satisfies (2.1) and has the representation

$$E = \sum_{i=0}^{k_0} \alpha_i z_i z_i' \tag{3.1}$$

where $z_1, \ldots, z_{k_0}$ are normalized eigenvectors ($||z_i||_2 = 1$) corresponding to the minimum eigenvalue $\lambda_{\min}$ of $M(\xi_E)$ and the α_i are positive numbers with sum 1. The following auxiliary result shows that we can always assume that the vectors $z_1, \ldots, z_{k_0}$ in this representation are linearly independent.

Lemma 3.1. Let ξ_E denote the E-optimal design and let E denote a matrix which satisfies the conditions of the equivalence Theorem 2.1. There exists a representation of E of the form (3.1) such that the vectors $z_1, \ldots, z_{k_0}$ are linearly independent.

Proof: Letting $k_0 = \text{rank}\ (E)$ we obtain for E the representations

$$E = \sum_{i=1}^{k} \alpha_i z_i z_i' \quad \text{and} \quad E = \sum_{i=1}^{k_0} \rho_i \rho_i'$$

where the first one follows from Theorem 2.1 and the second from the eigenvalue decomposition of the non-negative definite matrix E (note that $\rho_1, \ldots, \rho_{k_0}$ are linearly independent). Let x denote a vector with $z_i' x = 0$ $(i = 1, \ldots, k)$. From the identity

$$0 = \sum_{i=1}^{k} \alpha_i (x' z_i)(z_i' x) = x' E x = \sum_{i=1}^{k_0} (\rho_i' x)^2$$

we conclude

$$\text{nullspace}\ \{z_1, \ldots, z_k\} \subseteq \ \text{nullspace}\ \{\rho_1, \ldots, \rho_{k_0}\}$$

or equivalently

$$\text{span}\ \{\rho_1, \ldots, \rho_{k_0}\} \subseteq \ \text{span}\ \{z_1, \ldots, z_k\}.$$

This shows that $\rho_1, \ldots, \rho_{k_0}$ are eigenvectors of $M(\xi_E)$ corresponding to $\lambda_{\min}$. From Theorem 2.1 we have $||z_i||_2 = 1$ and $\sum_{i=1}^{k} \alpha_i = 1$ which implies

$$\sum_{i=1}^{k_0} ||\rho_i||_2^2 = trE = \sum_{i=1}^{k} \alpha_i ||z_i||_2^2 = 1.$$

Therefore

$$E = \sum_{i=1}^{k_0} ||\rho_i||_2^2 \left(\frac{\rho_i}{||\rho_i||_2} \right) \left(\frac{\rho_i}{||\rho_i||_2} \right)'$$

is a representation of E of the form (3.1) with linearly independent eigenvectors of $M(\xi_E)$ corrseponding to the minimum eigenvalue $\lambda_{\min}$.

In what follows we will always assume a representation of E by linearly independent eigenvectors $z_1, \ldots, z_{k_0}$. Note that k_0 is not necessary the multiplicity of $\lambda_{\min}$ and that $k_0 \leq n$. For these representations we have the following result.

Theorem 3.2. Let ξ_E denote the E-optimal design and E denote the matrix in the equivalence Theorem 2.1 with a linearly independent representation of the form (3.1). Then the design ξ_E is optimal for $A'\theta$ where $A = (\sqrt{\alpha_1} z_1, \ldots, \sqrt{\alpha_{k_0}} z_{k_0}) \in \mathbb{R}^{n \times k_0}$.

Proof: Let $E = \sum_{i=1}^{k_0} \alpha_i z_i z_i'$ denote a representation of the matrix E where $z_1, \ldots, z_{k_0}$ are linearly independent eigenvectors of $M(\xi_E)$ corresponding to $\lambda_{\min}$. From Theorem 2.1 we obtain for all $x \in \mathcal{X}$

$$\lambda_{\min} \geq f'(x)Ef(x) = f'(x) \sum_{i=1}^{k_0} (\sqrt{\alpha_i} z_i)(\sqrt{\alpha_i} z_i)' f(x) = tr(f'(x)AA'f(x))$$

where $A = (\sqrt{\alpha_1} z_1, \ldots, \sqrt{\alpha_{k_0}} z_{k_0}) \in \mathbb{R}^{n \times k_0}$ has rank k_0. Because we are interested in the E-optimal design for the whole parameter vector we may assume that $M(\xi_E)$ is positive definite which yields (note that $M(\xi_E) z_i = \lambda_{\min} z_i$)

$$\lambda_{\min} \geq tr(A'f(x)f'(x)A) = \lambda_{\min}^2 tr(A'M^{-1}(\xi_E)f(x)f'(x)M^{-1}(\xi_E)A).$$

Therefore we have for all $x \in \mathcal{X}$ (note $||z_i||_2 = 1$)

$$tr(A'M^{-1}(\xi_E)f(x)f'(x)M^{-1}(\xi_E)A) \leq \frac{1}{\lambda_{\min}} = \sum_{i=1}^{k_0} \alpha_i z_i' M^{-1}(\xi_E) z_i$$
$$= \sum_{i=1}^{k_0} \alpha_i tr(M^{-1}(\xi_E) z_i z_i') = tr(M^{-1}(\xi_E)AA')$$

and it follows from Theorem 2.2 that the design ξ_E is optimal for $A'\theta$ where $A = (\sqrt{\alpha_1} z_1, \ldots,$ $\sqrt{\alpha_{k_0}} z_{k_0})$.

Remark: Reversing the above steps one can easily obtain a converse to Theorem 3.2. That is, suppose that the design ξ_A is optimal for $A'\theta$ where $A = (\sqrt{\alpha_1} z_1, \ldots, \sqrt{\alpha_{k_0}} z_{k_0})$ for some set $\{\alpha_i\}_{i=1}^{k_0}$ $\left(\sum_{i=1}^{k_0} \alpha_i = 1\right)$ and $z_1, \ldots, z_{k_0}$ are linearly independent normalized eigenvectors corresponding to $\lambda_{\min}(M(\xi_A)) > 0$. Then the design ξ_A is also E-optimal and a matrix E in the representation (2.1) of Theorem 2.1 is given by $E = \sum_{i=1}^{k_0} \alpha_i z_i z_i'$.

The above result is the basic step for a discussion of the geometric characterization of E-optimality according to Elfving's Theorem 2.3. Recalling the definition of the Elfving set in (2.2) we obtain that there exists a number $\gamma > 0$ and vectors $\varepsilon_1', \ldots, \varepsilon_m'$ such that for the E-optimal design $\xi = \left\{ \begin{smallmatrix} x_i \\ p_i \end{smallmatrix} \right\}_{i=1}^{m}$ the point

$$\gamma A = \sum_{i=1}^{m} p_i f(x_i) \varepsilon_i' \tag{3.2}$$

lies on the boundary of the set $\mathcal{R}_{k_0}$ where k_0 is the number of eigenvectors in the representation (3.1) and $A = (\sqrt{\alpha_1} z_1, \ldots, \sqrt{\alpha_{k_0}} z_{k_0}) \in \mathbb{R}^{n \times k_0}$ is the matrix of Theorem 3.2. Moreover we have for the number γ from (2.5)

$$\gamma^{-2} = tr(M^{-1}(\xi_E)AA') = \frac{1}{\lambda_{\min}} \tag{3.3}$$

and for the supporting hyperplane D at the point $\gamma A = \sqrt{\lambda_{\min}} A$ from Lemma 2.4 and (2.4)

$$(3.4) \qquad \begin{cases} D = \gamma M^{-1}(\xi_E) A = \frac{1}{\sqrt{\lambda_{\min}}} A \\ \varepsilon_i = D' f(x_i) = \frac{1}{\sqrt{\lambda_{\min}}} A f(x_i) \quad i = 1, \ldots, m. \end{cases}$$

The equations (3.2) and (3.4) show that the boundary point $\sqrt{\lambda_{\min}} A \in \partial \mathcal{R}_{k_0}$ and its supporting hyperplane D at $\mathcal{R}_{k_0}$ have the same direction. This suggests that the boundary point $\sqrt{\lambda_{\min}} A$ is an inball vector of the Elfving set $\mathcal{R}_{k_0} \subseteq \mathbb{R}^{n \times k_0}$ which means that the norm of $\sqrt{\lambda_{\min}} A$ attains the minimum distance to the origin

$$r_{k_0} = \min\{||x||_2 | x \in \partial \mathcal{R}_{k_0}\}$$

among all boundary points of $\mathcal{R}_{k_0}$.

Theorem 3.3. Let ξ_E denote the E-optimal design, E a matrix which satisfies the conditions of Theorem 2.1 with a linearly independent representation (3.1) and define the matrix $A_k = (\sqrt{\alpha_1} z_1, \ldots, \sqrt{\alpha_{k_0}} z_{k_0}, 0, \ldots, 0) \in \mathbb{R}^{n \times k}$ $(k_0 \leq k \leq n)$ where the last $k - k_0$ columns of A_k contain only zeros. Then the point $\sqrt{\lambda_{\min}} A_k$ is an inball vector of the set $\mathcal{R}_k$ for any $k \geq k_0$ and we have $r_k^2 = \lambda_{\min}$ for all $k \geq k_0$.

Proof: From (3.2) and (3.3) we have that the matrix $\sqrt{\lambda_{\min}} A_{k_0}$ is a boundary point of $\mathcal{R}_{k_0}$ with supporting hyperplane D given by (3.4). By Lemma 2.4 $\sqrt{\lambda_{\min}} A_k$ is a boundary point of $\mathcal{R}_k$ with supporting hyperplane $D_k = (D, 0, \ldots, 0) \in \mathbb{R}^{n \times k}$ for any $k \geq k_0$. For the norm of A_k we obtain

$$||A_k||_2^2 = tr(A_k A_k') = \sum_{i=1}^{k_0} \alpha_i z_i' z_i = 1$$

which implies $(\sqrt{\lambda_{\min}} A_k \in \partial \mathcal{R}_k)$

$$(3.5) \qquad r_k^2 \leq ||\sqrt{\lambda_{\min}} A_k||_2^2 = \lambda_{\min} \text{ for all } k \geq k_0.$$

On the other hand we have for every $D \in \mathbb{R}^{n \times k}$ with $||D' f(x)||_2 \leq 1$ (for all $x \in \mathcal{X}$) that $tr(D' M(\xi) D) \leq 1$ for every design ξ on $\mathcal{X}$. This implies that

$$\frac{1}{\lambda_{\min}} = \inf_{\xi} \sup_{F} \frac{tr(M^{-1}(\xi) F F')}{tr F F'} = \inf_{\xi} \sup_{F} \sup_{G} \left\{ \frac{tr^2(G' F)}{tr(G' M(\xi) G)} \frac{1}{tr(F F')} \right\}$$
$$\geq \inf_{\xi} \sup_{F} \frac{tr^2(D' F)}{tr(D' M(\xi) D)} \frac{1}{tr(F F')} \geq \sup_{F} \frac{tr^2(D' F)}{tr(F F')} = tr(D' D).$$

Here we have used the identity $tr(M^{-1}FF') = \sup_G(tr^2 G'F/tr(G'MG))$ (see Studden (1971) p. 1614) which follows from the Cauchy Schwarz inequality, as does the last step. Because the distance from the hyperplane D to the origin is given by $1/tr(D'D)$ we obtain for the squared inball radius the representation

$$r_k^2 = \inf\left\{\frac{1}{tr(D'D)}\middle| D \in \mathbb{R}^{n\times k}, ||D'f(x)||_2 \le 1 \quad \forall\, x \in \mathcal{X}\right\}. \tag{3.6}$$

Thus we have $r_k^2 \ge \lambda_{\min}(k \ge k_0)$ which in combination with (3.5) proves the assertion of the theorem.

Theorem 3.3 can roughly be summarized in the following way. Considering the Elfving sets $\mathcal{R}_1, \mathcal{R}_2, \mathcal{R}_3, \ldots$ there exists a number k_0 such that all squared inball radii r_k^2 are equal to the minimum eigenvalue of the E-optimal design for $k \ge k_0$. In every set $\mathcal{R}_k(k \ge k_0)$ there exists at least one inball vector $\sqrt{\lambda_{\min}}A \in \mathbb{R}^{n\times k}$ for which the E-optimal design is also optimal for $A'\theta$. From the linear independence of the vectors $z_1, \ldots, z_{k_0}$ in the representation (3.1) we obtain that $k_0 \le n$. This suggests the following procedure for the determination of E-optimal designs. Look at the inball vectors A of the set $\mathcal{R}_n$ (because we do not know the number $k_0 \le n$ in the representation (3.1)) and determine the optimal designs for $A'\theta$ by known results for this optimality criterion. However, some caution is appropriate in the application of this procedure for the determination of E-optimal designs as indicated in the following example.

Example Let $n = 2, f(x) = (x_1, x_2)', \mathcal{X} = \left\{\binom{1}{1}, \binom{1}{-1}, \binom{1/2}{1}, \binom{-1/2}{1}\right\}$, it can easily be shown that $r_1^2 = r_2^2 = 1 = \lambda_{\min}$ (note that $n = 2$ implies $r_2^2 = \lambda_{\min}$). Because $A = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$ is a boundary point of $\mathcal{R}_2$ with supporting hyperplane $D = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$ we see that A is an inball vector of $\mathcal{R}_2$. By the representation (note that $\varepsilon_i' = f'(x_i)D$ by Lemma 2.4)

$$A = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} \frac{1}{2} \\ 1 \end{pmatrix}(1,0) + \frac{1}{2}\begin{pmatrix} -\frac{1}{2} \\ 1 \end{pmatrix}(1,0)$$

we obtain from the (Elfving) Theorem 2.3 that the design which puts equal mass at the points $\binom{\frac{1}{2}}{1}$ and $\binom{-\frac{1}{2}}{1}$ is optimal for $A'\theta$ where A is an inball vector of $\mathcal{R}_2$. Its information matrix and its minimum eigenvalue are given by

$$M(\xi_A) = \begin{pmatrix} \frac{1}{4} & 0 \\ 0 & 1 \end{pmatrix}, \lambda_{\min}(M(\xi_A)) = \frac{1}{4} < \lambda_{\min}$$

and therefore the design ξ_A is not the E-optimal one. On the other hand, we have for A the representation

$$A = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}(1,0) + \frac{1}{2}\begin{pmatrix} 1 \\ -1 \end{pmatrix}(-1,0)$$

which shows that the design ξ_E which puts equal mass at $\binom{1}{1}$ and $\binom{1}{-1}$ is also optimal for $A'\theta$. It is easily verified that this design is the E-optimal one.

The above example shows that not every optimal design for $A'\theta$ (where A is an inball vector of $\mathcal{R}_n$) is necessarily an E-optimal design. However, by Theorem 3.3 there always exists an inball vector A of $\mathcal{R}_k$ such that the corresponding optimal design for $A'\theta$ is E-optimal. The following theorem shows that the E-optimal design is optimal for $A'\theta$ for every inball vector A of the set $\mathcal{R}_k (k \geq k_0)$.

Theorem 3.4. Let ξ_E denote the E-optimal design and E the corresponding matrix of Theorem 2.1 with a representation (3.1) of k_0 linearly independent vectors $z_1, \ldots, z_{k_0}$. Whenever $n \geq k \geq k_0$ and $\sqrt{\lambda_{\min}}A$ is any inball vector of $\mathcal{R}_k$ the E-optimal design is also optimal for $A'\theta$ (or equivalently for $\sqrt{\lambda_{\min}}A'\theta$).

Moreover, if $D \in \mathbb{R}^{n \times k}$ is a supporting hyperplane of $\mathcal{R}_k$ at $\sqrt{\lambda_{\min}}A$, we have $||D'f(x_i)||_2 = 1$ for all support points x_i of the E-optimal design.

Proof: Because $\sqrt{\lambda_{\min}}A$ is an inball vector of $\mathcal{R}_k$ and $k \geq k_0$ we have from Theorem 3.3

$$\lambda_{\min} = r_k^2 = tr(\sqrt{\lambda_{\min}}AA'\sqrt{\lambda_{\min}}) = \lambda_{\min} trAA'$$

which implies $trAA' = 1$. Let ξ_A denote an optimal design for $A'\theta$, then we obtain from (Elfving's) Theorem 2.3 and (2.5)

$$\frac{1}{\lambda_{\min}} = tr(A'M^{-}(\xi_A)A) = \inf_{\xi} tr(A'M^{-}(\xi)A).$$

On the other hand it follows for the E-optimal design ξ_E that

$$\begin{aligned} \frac{1}{\lambda_{\min}} &= \inf_{\xi} tr(A'M^{-}(\xi)A) \leq tr(A'M^{-1}(\xi_E)A) \\ &= \frac{tr(A'M^{-1}(\xi_E)A)}{tr(AA')} \leq \sup_A \frac{tr(A'M^{-1}(\xi_E)A)}{tr(AA')} = \frac{1}{\lambda_{\min}} \end{aligned}$$

which shows that ξ_E is also optimal for $A'\theta$ (because $tr(A'M^{-1}(\xi_E)A)$ attains the optimal value $1/\lambda_{\min}$).

If D is a supporting hyperplane of $\mathcal{R}_k$ at $\sqrt{\lambda_{\min}}A$ it follows from $||D'f(x)||_2 \leq 1$ that $tr(D'M(\xi)D) \leq 1$ for any design ξ on $\mathcal{X}$ and we obtain

$$\frac{1}{\lambda_{\min}} = tr(A'M^{-1}(\xi_E)A) = \sup_F \frac{tr^2(F'A)}{tr(F'M(\xi_E)F)}$$
$$\geq \frac{tr^2(D'A)}{tr(D'M(\xi_E)D)} \geq tr^2(D'A) = \frac{1}{\lambda_{\min}}.$$

Thus we have $1 = tr(D'M(\xi_E)D) = \sum_{i=1}^{m} p_i tr(D'f(x_i)f'(x_i)D) \leq 1$ which shows $||D'f(x_i)||_2 = 1$ for all support points x_i of the E-optimal design.

The results derived so far suggest the following procedure for the determination of the E-optimal design. First the inball radius of $\mathcal{R}_n$, an inball vector A and its supporting hyperplane D have to be found. From Theorem 3.3 we know the existence of $k_0 \leq n$ such that $r_k^2 = \lambda_{\min}$ for all $k \geq k_0$ which shows that the squared inball radius of $\mathcal{R}_n$ is given by the minimum eigenvalue of the E-optimal design. In a second step we have to find the designs which are optimal for $A'\theta$ and calculate the minimum eigenvalue of the corresponding moment matrices. Any design whose minimum eigenvalue is equal to the inball radius of $\mathcal{R}_n$ is, of course, E-optimal. Theorem 3.4 says that the E-optimal design has to be among these designs and that all support points x_i satisfy $||D'f(x_i)||_2 = 1$. Moreover if there are several inball vectors $A_j (j \in I)$ of $\mathcal{R}_n$ with supporting hyperplanes D_j we have for the support of the E-optimal design

$$\text{supp}\,(\xi_E) = \bigcap_{j \in I} \{x | \; ||D_j x||_2 = 1\}.$$

(There actually may be more than one supporting hyperplane D_j for a given inball vector A_j.) We will demonstrate this procedure in some examples in section 4. The main step is the determination of the inball radius of $\mathcal{R}_n$. The following result gives estimates of the inball radius r_m by the inball radius $r_k (m \leq k)$ and is often very useful for the calculation of the inball radii of $\mathcal{R}_k$.

Theorem 3.5. Let r_k denote the inball radius of $\mathcal{R}_k (k = 1, \ldots, n)$ and $\lambda_{\min}$ denote the minimum eigenvalue of the E-optimal design.

a) The sequence $r_1, r_2, r_3, \dots$ is decreasing

b) $r_k^2 \geq \lambda_{\min}$ for all $1 \leq k \leq n$

c) For all $m \leq k \leq n$ we have $mr_m^2 \leq kr_k^2$

Proof: Let $A_k \in \mathbb{R}^{n\times k}$ denote an inball vector of $\mathcal{R}_k$ with supporting hyperplane D_k, then the point $A_{k+1} = (A_k, 0) \in \mathbb{R}^{n\times k+1}$ is also a boundary point of $\mathcal{R}_{k+1}$ with supporting hyperplane $D_{k+1} = (D_k, 0) \in \mathbb{R}^{n\times k+1}$ (by Lemma 2.4). This implies

$$r_{k+1}^2 \leq tr(A_{k+1}A'_{k+1}) = tr(A_k A'_k) = r_k^2$$

which proves part a). By Theorem 3.3 we find $r_n^2 = \lambda_{\min}$ and thus a) implies b). To prove c) let $D = (d_1, \dots, d_k) \in \mathbb{R}^{n\times k}$ be a matrix such that $||D'f(x)||_2 \leq 1$ for all $x \in \mathcal{X}$, then we have for any subset $I \subseteq \{1, \dots, k\}$ with $\#I = m \leq k$

$$1 \geq ||D'f(x)||_2^2 = \sum_{i=1}^{k} (d_i' f(x))^2 \geq \sum_{i\in I} (d_i' f(x))^2.$$

Therefore $D_I = (d_{i_1}, \dots, d_{i_m}) \in \mathbb{R}^{n\times m}$ fulfills $||D_I' f(x)||_2 \leq 1$ for all $x \in \mathcal{X}$ and all $I = \{i_1, \dots, i_m\} \subseteq \{1, \dots, k\}$. Thus D_I is a supporting hyperplane of $\mathcal{R}_m$ and (3.6) implies

$$r_m^2 \leq \frac{1}{tr(D_I D_I')} = \left(\sum_{i\in I} d_i' d_i\right)^{-1}.$$

From this inequality we obtain

$$\sum_{i=1}^{k} d_i' d_i = \frac{1}{\binom{k-1}{m-1}} \left(\sum_{\substack{I\subseteq\{1,\dots,k\} \\ \#I=m}} \sum_{i\in I} d_i' d_i \right) \leq \frac{1}{\binom{k-1}{m-1}} \sum_{\substack{I\subseteq\{1,\dots,k\} \\ \#I=m}} \frac{1}{r_m^2}$$
$$= \frac{\binom{k}{m}}{\binom{k-1}{m-1}} \frac{1}{r_m^2} = \frac{k}{m} \frac{1}{r_m^2}$$

which proves part c) of the theorem.

We should mention at this point that the bounds of b) and c) are sharp. More precisely we will present two examples in section 4 for which $\lambda_{\min}$ has multiplicity n and we have equality in b) or c).

Although the calculation of the inball radii r_k is not always possible in general we can usually find upper bounds for r_k by identifying some boundary points of $\mathcal{R}_k$. These bounds can be used as bounds in the E-efficiency calculation of a given design. For example if $c \geq r_k$ for some k we obtain for the E-efficiency Eff (ξ) of a design ξ from Theorem 3.5 b)

$$\text{(3.7)} \qquad \text{Eff }(\xi) = \frac{\lambda_{\min}(M(\xi))}{\lambda_{\min}} \geq \frac{\lambda_{\min}(M(\xi))}{r_k^2} \geq \frac{\lambda_{\min}(M(\xi))}{c^2}.$$

We will finish this section by giving a bound of the multiplicity of the minimum eigenvalue of the E-optimal design which can be determined from the sequence of inball radii $(r_1, r_2, \ldots, r_n)$.

Corollary 3.6 Let r_k denote the inball radius of $\mathcal{R}_k$ and $f = \max\{i | r_i < r_{i-1}\}$ (if $r_1 = r_2 = \ldots = r_n$ define $f = 1$) then the multiplicity of the minimum eigenvalue of the E-optimal design is greater or equal f.

Proof: Let E denote the matrix of the equivalence Theorem 2.1 with a linearly independent representation (3.1). From Theorem 3.3 we have $r_{k_0} = r_{k_0+1} = \ldots = r_n$ which implies $f \leq k_0 \leq$ multiplicity of $\lambda_{\min}$.

4. Examples.

1) Spring balance weighing designs. In a recent paper Cheng (1987) investigated Φ_p-optimal designs for the following regression setup $f(x) = x = (x_1, x_2, \ldots, x_n)', \mathcal{X} = \{0,1\}^n$. These designs are called spring balance weighing designs (see Raghavarao (1971), chapter 17). Cheng (1987) applied an equivalence theorem of Kiefer (1974) and determined the Φ_p-optimal approximate designs. For $p = \infty$ he found the E-optimal spring balance weighing design. By the application of our results we can present an elementary (geometric) solution of this E-optimal design problem. To this end let $\mathcal{R}_k^n$ denote the Elfving set of Theorem 2.3 and $r_k(n)$ the corresponding inball radius (here the index n represents the number of regression functions). Let $D' = (d_1, \ldots, d_n) \in \mathrm{R}^{k \times n}$ denote a matrix satisfying $||D'f(x)||_2 \leq 1$ for all $x \in \mathcal{X}$ (note that in contrast to section 3 the vectors $d_1, \ldots, d_n$ denote here the columns of D'). For the determination of the inball radius $r_k(n)$ of $\mathcal{R}_k^n (k \leq n)$ we have to solve the problem (see (3.6))

$$\text{(5.1)} \qquad \text{Minimize } \frac{1}{tr(DD')} \text{ subject to } ||D'x||_2 \leq 1 \;\; \forall \, x \in \mathcal{X}.$$

Inserting all possible points $x \in \mathcal{X} = \{0,1\}^n$ in the constraint (5.1) is equivalent to the problem

$$\text{Maximize } \sum_{i=1}^{n} ||d_i||_2^2 \text{ subject to } ||\sum_{i\in I} d_i||_2 \leq 1 \text{ for all } I \subseteq \{1,\dots,n\}$$

which has the following nice geometric interpretation: "In the set of n vectors $\{d_1,\dots,d_n\}$ in the unit ball B of $\mathbb{R}^k$ such that the sum of any of these vectors is also contained in B maximize the sum of the squared norms of all n vectors". For the solution of this problem it is convenient to distinguish the case $n = 2m$ and $n = 2m+1$. We consider at first the even case and $k = 2m$ which is the interesting case for E-optimality. The matrix $D' = (d_1,\dots,d_n)$ has to satisfy the conditions

$$\sum_{i\in I} ||d_i||_2^2 + \sum_{i\in I} \sum_{\substack{j\in I \\ i\neq j}} d_i' d_j = ||\sum_{i\in I} d_i||_2^2 \leq 1 \tag{5.2}$$

for all subsets $I \subseteq \{1,\dots,2m\}$. Considering only the subsets I with exactly m elements and adding the inequalities of (5.2) corresponding to these sets we obtain

$$\binom{2m-1}{m-1} \sum_{i=1}^{2m} ||d_i||_2^2 + \frac{\binom{2m}{m}\binom{m}{2}}{\binom{2m}{2}} \sum_{i=1}^{2m} \sum_{\substack{j=1 \\ j\neq i}}^{2m} d_i' d_j \leq \binom{2m}{m}. \tag{5.3}$$

From $||\sum_{i=1}^{2m} d_i||_2^2 \geq 0$ it follows that

$$\sum_{i=1}^{2m} \sum_{\substack{j=1 \\ j\neq i}}^{2m} d_i' d_j \geq - \sum_{i=1}^{2m} ||d_i||_2^2$$

and (5.3) reduces after some algebra to

$$tr(DD') = \sum_{i=1}^{2m} ||d_i||_2^2 \leq \frac{2(2m-1)}{m}. \tag{5.4}$$

On the other hand it is easy to verify that the matrix

$$D_0 = \frac{1}{\sqrt{2m^3}} \begin{pmatrix} 2m-1 & -1 & \dots & -1 \\ -1 & 2m-1 & \dots & -1 \\ \vdots & & \ddots & \vdots \\ -1 & -1 & \dots & 2m-1 \end{pmatrix} \in \mathbb{R}^{2m\times 2m}$$

satisfies $||D_0'x||_2^2 \leq 1$ for all $x \in \{0,1\}$ and that $trD_0D_0' = \frac{2(2m-1)}{m}$. This shows that D_0 is a solution of the problem (5.1) and that the inball radius $r_{2m}(2m)$ of $\mathcal{R}_{2m}^{2m}$ and the minimum eigenvalue of the E-optimal design are given by (see Theorem 3.3)

$$\lambda_{\min} = r_{2m}^2(2m) = \frac{m}{2(2m-1)}.$$

The inball vector of $\mathcal{R}_{2m}^{2m}$ is given by $\sqrt{\lambda_{\min}}A = \frac{m}{2(2m-1)}D_0$ with supporting hyperplane D_0 and by Theorem 3.4 we obtain that the support of the E-optimal design is included in the set

$$\{x|\ ||D_0'x||_2 = 1\} = \{x \in \{0,1\}^{2m}|\ x \text{ has exactly } m \text{ components equal } 1\}.$$

Let $\{v_i\}$ denote the set of vectors in $\mathbb{R}^{2m}$ with m components 0 and m components 1, then it is straight forward to show that the design ξ_E which puts uniform mass on the $\binom{2m}{m}$ vectors v_i has information matrix $M(\xi_E) = \frac{m}{2(2m-1)}I_{2m} + \frac{m-1}{2(2m-1)}J_{2m}$ with minimum eigenvalue $\lambda_{\min} = \frac{m}{2(2m-1)}$ (here I_{2m} denotes the identity matrix and J_{2m} the matrix with all elements equal 1). Therefore ξ_E is the E-optimal spring balance weighing (approximate) design (for $n = 2m$) and the minimum eigenvalue $\lambda_{\min}$ has multiplicity $2m-1$. By the same reasoning it can be shown that for $n = 2m+1$ the E-optimal design puts equal mass at the $\binom{2m+1}{m}$ vertices of $[0,1]^{2m+1}$ with $m+1$ coordinates equal 1 and m coordinates equal 0. The minimum eigenvalue is $r_{2m+1}^2(2m+1) = \lambda_{\min} = \frac{m+1}{2(2m+1)}$ and has multiplicity $2m$.

For the determination of the E-optimal design it is sufficient to look at the set $\mathcal{R}_n^n$ and its corresponding inball radius $r_n(n)$. However for the illustration of the theorems of section 3 it might be useful to investigate also the inball radii $r_k(n)$ for $k < n$ in this example. At first we will show that the inball radius of the set $\mathcal{R}_{n-1}^n$ is the same as for $\mathcal{R}_n^n$. For this purpose we consider again only the case of $n = 2m$ even. Because the derivation of (5.4) does not depend on the dimension of the vectors d_i we still have $r_{2m-1}^2(2m) \geq \frac{m}{2(2m-1)}$. Let $\tilde{D}_0 = (\tilde{d}_1, \ldots, \tilde{d}_{2m-1}) \in \mathbb{R}^{2m \times 2m-1}$ where

$$\tilde{d}_i = \frac{\sqrt{2}}{\sqrt{m}} \frac{\sqrt{2m-i}}{\sqrt{2m-i+1}} (\underbrace{0,\ldots,0}_{i-1}, 1, \underbrace{-\frac{1}{2m-i}, \ldots, -\frac{1}{2m-i}}_{2m-i})' \in \mathbb{R}^{2m}$$

($i = 1, \ldots, 2m-1$) then its straightforward to check that $\tilde{D}_0$ fulfills $||\tilde{D}_0'x||_2 \leq 1$ for all $x \in \mathcal{X}$ and

$$tr(\tilde{D}_0\tilde{D}_0') = \sum_{i=1}^{2m-1} \tilde{d}_i'\tilde{d}_i = \frac{2(2m-1)}{m}.$$

This shows that the lower bound for $r_{2m-1}^2(2m)$ is attained and we have $r_{2m-1}^2(2m) = r_{2m}^2(2m) = \lambda_{\min}$. In the same way we can prove the case $n = 2m+1$ and obtain $r_{n-1}(n) = r_n(n)$ for all $n \geq 2$. In the next step we will show that $r_k(n) = r_k(k+1)$ for all $n \geq k+1$.

The inequality $r_k(n) \le r_k(k+1)$ is obvious (by the same reasoning as in the proof of Theorem 3.5 a)); for the converse inequality consider at first the case $k = 2m+1$. We have from the first part

$$r^2_{2m+1}(2m+2) = r^2_{2m+2}(2m+2) = \frac{m+1}{2(2m+1)} = r^2_{2m+1}(2m+1).$$

Now we consider the case $n = 2m+3$ and let $D' = (d_1, \dots, d_{2m+3}) \in \mathbb{R}^{2m+1 \times 2m+3}$ with $||D'x||_2 \le 1 \ \forall x \in \{0,1\}^{2m+3}$. It can easily be proved (by looking at the signs of the inner products) that the minimum of the angles between $n+2$ vectors in $\mathbb{R}^n$ is less or equal 90°. Therefore D' contains at least two vectors, say d_1 and d_2 with $d_1'd_2 \ge 0$. For the matrix $\tilde{D}' = (d_1 + d_2, d_3, \dots, d_{2m+3}, 0) \in \mathbb{R}^{2m+1 \times 2m+3}$ we verify that $||\tilde{D}'x||_2 \le 1$ (because all sums of the vectors of D' are in the unit ball of $\mathbb{R}^{2m+1}$ this is also fulfilled for the vectors of $\tilde{D}'$) and obtain

$$tr\tilde{D}'\tilde{D} = \sum_{i=1}^{2m+3} ||d_i||_2^2 + 2d_1'd_2 \ge \sum_{i=1}^{2m+3} ||d_i||_2^2 = trD'D.$$

The matrix $D_0' = (d_1 + d_2, d_3, \dots, d_{2m+3}) \in \mathbb{R}^{2m+1 \times 2m+2}$ can also be used for the calculation of $r_{2m+1}(2m+2)$ and we obtain from (3.6)

$$r^2_{2m+1}(2m+2) \le \frac{1}{tr(D_0'D_0)} = \frac{1}{tr(\tilde{D}'\tilde{D})} \le \frac{1}{tr(D'D)}$$

for all matrices $D \in \mathbb{R}^{2m+3 \times 2m+1}$ satisfying $||D'x||_2 \le 1$ $(x \in \{0,1\}^{2m+3})$. This shows $r_{2m+1}(2m+2) \le r_{2m+1}(2m+3)$ and because the converse inequality is obvious we have $r_{2m+1}(2m+3) = r_{2m+1}(2m+2) = r_{2m+1}(2m+1)$. Repeating these arguments gives the desired result

$$r_{2m+1}(n) = r_{2m+1}(2m+1) \text{ for all } n \ge 2m+1. \tag{5.5}$$

For the case $k = 2m$ we apply Theorem 3.5 a) and obtain using (5.5)

$$r_{2m+1}(2m+1) = r_{2m}(2m+1) \ge r_{2m}(n) \ge r_{2m+1}(n) = r_{2m+1}(2m+1)$$

which shows $r_{2m}(n) = r_{2m}(2m+1)$ whenever $n \ge 2m+1$. Summarizing all results obtained so far we have for the squared inball radii $r_k^2(n)$ in the spring balance weighing design example

$$r_k^2(n) = \begin{cases} \frac{[\frac{n+1}{2}]}{2(2[\frac{n+1}{2}]-1)} = \lambda_{\min} & \text{for } k = n-1, n \\ r_k^2(n) = \lambda_{\min} & \text{for all } k \ge n \\ r_k^2(k+1) & \text{for all } n \ge k+1 \end{cases}$$

The squared inball radii are illustrated in Table 4.1 for $n \leq 7, k \leq 7$.

$k\backslash n$	1	2	3	4	5	6	7	...
1	1	1/2	1/2	1/2	1/2	1/2	1/2	...
2	1	1/2	1/3	1/3	1/3	1/3	1/3	...
3	1	1/2	1/3	1/3	1/3	1/3	1/3	...
4	1	1/2	1/3	1/3	3/10	3/10	3/10	...
5	1	1/2	1/3	1/3	3/10	3/10	3/10	...
6	1	1/2	1/3	1/3	3/10	3/10	2/7	...
7	1	1/2	1/3	1/3	3/10	3/10	2/7	...
	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋱

Table 4.1: The squared inball radii of the sets $\mathcal{R}_k^n$ $(n \leq 7, k \leq 7)$ for the spring balance weighing designs

We see that for fixed n the sequence of inball radii $(r_1, r_2, r_3, \ldots)$ is not strictly decreasing.

2) Chemical balance weighing design. Let $f(x) = x = (x_1, \ldots, x_n)', \mathcal{X} = \{-1, 0, 1\}^n$. These designs are called chemical balance weighing designs because they often occur in chemical weighing operations (see Raghavarao (1971)). We will use the results of section 3 and determine the E-optimal chemical balance weighing (approximate) design. To this end let $D' = (d_1, \ldots, d_n) \in \mathbb{R}^{k \times n}$ be a matrix satisfying $||D'x||_2^2 \leq 1$ for all $x \in \{-1, 0, 1\}^n$. Inserting in this inequalities all 2^{n-1} vectors of the form $(1, \varepsilon_2, \ldots, \varepsilon_n)' \in \{-1, 0, 1\}^n$ where $\varepsilon_i = \mp 1$ $(i = 2, \ldots, n)$ and adding these inequalities we obtain

$$2^{n-1} \sum_{i=1}^{n} d_i' d_i \leq 2^{n-1}$$

which gives the lower bound 1 for the inball radius $r_k(n)$ of $\mathcal{R}_k^n$. For $n \geq k$ define the matrix $D_0' = \left(\frac{1}{k} I_k, 0\right) \in \mathbb{R}^{k \times n}$, then we have $||D_0' x||_2^2 = \frac{1}{k} \sum_{i=1}^{k} x_i^2 \leq 1$ for all $x \in \mathcal{X}$ and $tr D_0' D_0 = 1$. Therefore D_0 attains the lower bound and we find $r_k(n) = 1$ for all k and $n \in \mathbb{N}$. The E-optimal chemical balance weighing design is obtained by an application of the necessary condition of Theorem 3.4 and puts equal masses at the 2^n points $(\mp 1, \ldots, \mp 1)' \in \mathbb{R}^n$. The minimum eigenvalue is 1 and has multiplicity n. This example shows that the bound in Theorem 3.5 b) cannot be improved. All squared inball radii $r_k(n) (k \leq n)$ are already equal to the minimum eigenvalue of the E-optimal design. The following example shows that equality can also occur in part c) of Theorem 3.5.

3) Linear regression without intercept on the n-ball. Let $f(x) = x = (x_1, \ldots, x_n)'$ and $\mathcal{X} = \{x \in \mathbb{R}^n | \ ||x||_2 \leq 1\}$. It is obvious that for all $n \in \mathbb{N}$ the "first" inball radius is given by $r_1(n) = 1$. From Theorem 3.5 part c) we thus obtain $(m = 1)$ $r_k^2(n) \geq \frac{r_1^2(n)}{k} = \frac{1}{k}$ for all $1 \leq k \leq n$ as a lower bound for the (squared) inball radius $r_k^2(n)$. It is easy to verify that the matrix $D' = (I_k, 0) \in \mathbb{R}^{k \times n}$ satisfies $||D'x||_2^2 \leq 1$ for all $x \in \mathcal{X}$ and that it attains the lower bound $\frac{1}{k}$. This shows that $r_k^2(n) = \frac{1}{k}$ for all $1 \leq k \leq n$. For $k = n$ we obtain the minimum eigenvalue of the E-optimal design $\lambda_{\min} = \frac{1}{n}$ with multiplicity n (by Corollary 3.6). It is straightforward that the design which puts uniform mass at the unit vectors $e_i = (0, \ldots, 0, 1, 0, \ldots, 0)'$ is a E-optimal design. In this example we have $mr_m^2 = kr_k^2 = 1$ for all $m \leq k \leq n$, i.e. equality in Theorem 3.5, part c).

4) Linear regression regression without intercept on the n-ball in the ℓ_p-norm. The following example is more of mathematical interest than of practical interest compared to the previous examples which arise in various applications of linear regression. Let $f(x) = x = (x_1, \ldots, x_n)'$, the design space is $\mathcal{X} = \{x | \ ||x||_p \leq 1\}$ where $||x||_p = \left(\sum_{i=1}^{n} |x_i|^p\right)^{1/p}$ denotes the ℓ_p-norm on $\mathbb{R}^n$ $(1 \leq p \leq \infty)$. In the previous example we have found the E-optimal design and all inball radii $r_k(n)$ for $p = 2, p = \infty$. We will now determine the E-optimal design for any $p \geq 1$. It is convenient to distinguish the cases $1 \leq p \leq 2$ and $2 \leq p \leq \infty$ and we will begin with the first one. Let $D' = (d_1, \ldots, d_n) \in \mathbb{R}^{n \times n}$ such that $||D'x||_2 \leq 1$ for all $x \in \mathcal{X}$. Inserting the unit vectors $e_i = (0, \ldots, 0, 1, 0, \ldots, 0)' \in \mathbb{R}^n$ in this inequality and adding these inequalities we obtain $\sum_{i=1}^{n} d_i' d_i \leq n$ which shows that $1/n$ is a lower bound for the (squared) inball vector $r_n^2(n)$, i.e. $r_n^2(n) \geq \frac{1}{n}$. For the matrix $D = I_n$ we have (note that $p \leq 2$)

$$||Dx||_2 = ||x||_2 \leq ||x||_p \leq 1 \text{ and } trD'D = \frac{1}{n}$$

which shows that $r_n^2(n) = \frac{1}{n}$. From Theorem 3.3 and 3.4 we conclude that $\lambda_{\min} = \frac{1}{n}$ and by straightforward arguments it can be shown that the E-optimal design puts equal masses at the points e_i $(i = 1, \ldots, n)$.

The case $p \geq 2$ is treated similar to example 2. We consider the 2^{n-1} vectors of the form $y = n^{-1/p}(1, \mp 1, \ldots, \mp 1) \in \mathcal{X}$. By a summation of all inequalities of the form $||D'y||_2^2 \leq 1$ we obtain

$$2^{n-1} n^{-\frac{2}{p}} \sum_{i=1}^{n} d_i' d_i \leq 2^{n-1}$$

which shows $r_n^2(n) \geq n^{-2/p}$. To prove equality we have to find a matrix D with $||D'x||_2 \leq 1$ and $trDD' = n^{2/p}$. The last equation is obviously fulfilled for the matrix $D_0 = n^{1/p-1/2}I_n$. On the other hand we see from $\left(\frac{1}{p}+\frac{1}{q}=1\right)$

$$||D_0'x||_2^2 = n^{\frac{2}{p}-1}||x||_2^2 = n^{\frac{2}{p}-1}\sum_{i=1}^n x_i^2$$
$$\leq n^{\frac{2}{p}-1}\left(\sum_{i=1}^n |x_i|^p\right)^{\frac{1}{p}}\left(\sum_{i=1}^n |x_i|^q\right)^{\frac{1}{q}} \leq ||x||_p^2 \leq 1$$

that D_0 satisfies also the other condition. Here we have used the inequality $n^{\frac{2}{p}-1}||x||_q \leq ||x||_p$ for $p \geq 2$ which is an elementary consequence of the Hölder inequality. Therefore the minimum eigenvalue of the E-optimal design is given by $\lambda_{\min} = r_n^2(n) = n^{-2/p}$. To identify the design itself we apply Theorem 3.4 and obtain that the design which puts equal masses at the points $n^{-1/p}(\mp 1, \mp 1, \ldots, \mp 1)$ is E-optimal if $p \geq 2$. Note that in the case $p = 2$ there may exist E-optimal designs with different support points than the points given above. This is a consequence of the fact, that for $p = 2$ the necessary condition $||D_0'x||_2 = 1$ of Theorem 3.4 reduces to $||x||_2 = 1$. An example for another E-optimal design is given in Example 3.

5) Cubic regression on the interval $[-b, b]$. Let $f(x) = (1, x, x^2, x^3)'$, $\mathcal{X} = [-b, b], b > 1$. In a recent paper Pukelsheim and Studden (1991) showed for the interval [-1, 1] that the minimum eigenvalue of the E-optimal design is given by $||c||_2^{-2}$ where $c'f(x) = T_3(x) = 4x^3 - 3x$ denotes the third Chebyshev polynomial of the first kind (these authors proved this statement for arbitrary degree and also identified the support of the E-optimal design on [-1, 1]). By an application of the results of section 3 we will show that this is not true on [-b, b] if b is sufficiently large. To this end we give estimates for the inball radii of the first two Elfving sets $\mathcal{R}_1$ and $\mathcal{R}_2$. Let $d = \left(0, -\frac{3}{b}, 0, \frac{4}{b^3}\right)'$, denote the vector of the coefficients of the third Chebyshev polynomial on $[-b, b]$, then we have for all $x \in [-b, b]$

$$||d'f(x)||_2^2 = \left(-3\frac{x}{b} + 4\left(\frac{x}{b}\right)^3\right)^2 = \left(T_3\left(\frac{x}{b}\right)\right)^2 \leq 1$$

which gives the upper bound (see (3.6))

$$\lambda_{\min} \leq r_1^2 \leq \left[\left(\frac{3}{b}\right)^2 + \left(\frac{4}{b^3}\right)^2\right]^{-1}. \tag{5.5}$$

For the determination of an upper bound for r_2 we remark, that it follows from the results of Dette (1992) that for any $\alpha \in [0,1]$ the matrix

$$D' = \begin{pmatrix} -\sqrt{\alpha(2-\alpha)} & 0 & \frac{2}{b^2}\sqrt{\alpha(2-\alpha)} & 0 \\ 0 & -\frac{3-\alpha}{b} & 0 & \frac{2(2-\alpha)}{b^3} \end{pmatrix}$$

satisfies the inequality

$$||D'f(x)||_2^2 = \alpha(2-\alpha)\left[-1+2\left(\frac{x}{b}\right)^2\right]^2 + \left[-(3-\alpha)\frac{x}{b} + 2(2-\alpha)\left(\frac{x}{b}\right)^3\right]^2 \leq 1$$

for all $x \in [-b, b]$ (this can also be verified directly checking that the above expression attains its maximum in $[-b, b]$ at the points $\mp b$ and $\mp\sqrt{\frac{1-\alpha}{2(2-\alpha)}}b$ and that this maximum is equal 1). Therefore we have

$$\text{(5.6)} \qquad \frac{1}{r_2^2} \geq g(\alpha) := tr(DD') = \alpha(2-\alpha)\left(1+\frac{4}{b^4}\right) + \frac{(3-\alpha)^2}{b^2} + \frac{4(2-\alpha)^2}{b^6}$$

for all $\alpha \in [0,1]$. By elementary calculations it can be shown that $g(\alpha)$ attains its maximum in [0, 1] at (note that $f''(\alpha) = -\frac{2}{b^6}(b^2-1)(b^4+4) < 0$ for all $b > 1$)

$$\alpha_{\max} = \begin{cases} \frac{b^6-3b^4+4b^2-8}{(b^2-1)(b^4+4)} & \text{if } b \geq b_0 \\ 0 & \text{if } b \leq b_0 \end{cases}$$

where $b_0 = 1.62307279$ and the maximum value is given by

$$f(\alpha_{\max}) = \begin{cases} \frac{b^8+3b^6+8b^4+12b^2+12}{b^2(b^2-1)(b^4+4)} & \text{if } b \geq b_0 \\ \left(\frac{3}{b}\right)^2 + \left(\frac{4}{b^3}\right)^2 & \text{if } b \leq b_0. \end{cases}$$

Here we have to distinguish the cases $b \geq b_0$ and $b \leq b_0$ because the solution of $f'(\alpha) = 0$ is not contained in the interval [0, 1] if $b \leq b_0$. From (5.6) we obtain the upper bound for r_2

$$\text{(5.7)} \qquad \lambda_{\min} \leq r_2^2 \leq \begin{cases} \frac{b^2(b^2-1)(b^4+4)}{b^8+3b^6+8b^4+12b^2+12} & \text{if } b \geq b_0 \\ \left[\left(\frac{3}{b}\right)^2 + \left(\frac{4}{b^3}\right)^2\right]^{-1} & \text{if } b \leq b_0. \end{cases}$$

Because $f(\alpha_{\max}) > f(0) = \left(\frac{3}{b}\right)^2 + \left(\frac{4}{b^3}\right)^2$ whenever $b > b_0$ we see from (5.7) that for $b > b_0$ the minimum eigenvalue of the E-optimal design is *not* given by $||d||_2^{-2}$ where $d = \left(0, -\frac{3}{b}, 0, \frac{4}{b^3}\right)$ denotes the vector of the coefficients of the third Chebyshev polynomial on $[-b,b]$ $\left(d'f(x) = T_3\left(\frac{x}{b}\right)\right)$. The same arguments will hold for polynomial regression of arbitrary degree $n \geq 2$ on $[-b,b]$.

The calculation of the inball radii for the cubic model on $[-b,b]$ (or general for the model of degree n) seems to be difficult because this problem is equivalent to a problem in nonlinear approximation theory. However, as mentioned in section 3 upper bounds of the inball radii r_k are very useful for the calculation of E-efficiences for a given design. As an illustration we consider the case $b = 3$ and obtain from (5.7)

$$\lambda_{\min} \leq r_2^2 \leq \frac{510}{793} = 0.6431$$

which gives the lower bound for the E-efficiency of a given design ξ (see (3.7))

$$\text{Eff }(\xi) = \frac{\lambda_{\min}(M(\xi))}{\lambda_{\min}} \geq \frac{793}{510} \cdot \lambda_{\min}(M(\xi)).$$

As an example we take the design η which puts masses proportional to 1:4:4:1 at the points -3, -1, 1, 3. The minimum eigenvalue of $M(\eta)$ is $\lambda_{\min}(M(\eta)) = 0.5881$ and its E-efficiency Eff $(\eta) \geq 91.44\%$. If we put masses proportional to 1:9:9:1 at the same points we obtain a minimum eigenvalue 0.6137 and a E-efficiency greater or equal 95.42%.

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