

## GEOMETRY OF $E$ -OPTIMALITY

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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 in-ball 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 in-ball 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 in-ball 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 in-ball 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.

**1. Introduction.** Let  $f(x) = (f_1(x), \dots, f_n(x))'$  denote  $n$  linearly independent regression functions on a compact set  $\mathcal{X}$  which contains at least  $n$  points and let  $\theta = (\theta_1, \dots, \theta_n)'$  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  $\xi$  defined on a  $\sigma$  field of sets of  $\mathcal{X}$  which include the one point sets. The information matrix of the design  $\xi$  is given by

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

If  $\xi$  concentrates mass  $n_i/N$  at the points  $x_i$ ,  $i = 1, \dots, r$ ,  $\sum_{i=1}^r n_i = N$ , the experimenter takes  $n_i$  uncorrelated observations at each  $x_i$ ,  $i = 1, \dots, r$ , and the covariance matrix of the least squares estimator of  $\theta$  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  $\xi$ . 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

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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  $\xi$  is called optimal for  $A'\theta$  if it minimizes  $\text{tr}(M^-(\xi)AA')$ , where  $M^-(\xi)$  denotes a generalized version of  $M(\xi)$  and  $\text{tr}(B)$  the trace of a matrix  $B$ . An optimal design for  $A'\theta$  can be used if the experimenter is interested in certain linear combinations  $a'_1\theta, \dots, a'_k\theta$  of the unknown parameter vector, where  $a_1, \dots, a_k$  denote the columns of the matrix  $A$ .

If the minimum eigenvalue of the  $E$ -optimal moment matrix has multiplicity 1, 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  $\xi$  is  $E$ -optimal if and only if it is optimal for  $a'_1\theta$ . Moreover, the vector  $\sqrt{\lambda_{\min}} a_1$  is an in-ball vector of the Elfving set

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

where  $\text{conv}(S)$  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 in-ball radius  $r_1$  and a corresponding in-ball 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 geometric 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 in-ball 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  $\xi_E$  is  $E$ -optimal [i.e., it maximizes the minimum eigenvalue of  $M(\xi)$ ] if and only if there exists a matrix  $E \in \text{conv}(S)$  such that*

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

Here  $\lambda_{\min}$  denotes the minimum eigenvalue of the matrix  $M(\xi_E) \in \mathbb{R}^{n \times n}$  and  $\text{conv}(S)$  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  $\xi_A$  denote a design for which  $\text{range}(A) \subseteq \text{range}(M(\xi_A))$ . The design  $\xi_A$  is optimal for  $A'\theta$  if and only if there exists a generalized inverse  $G$  of  $M(\xi_A)$  such that*

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

The following theorem was proved by Studden (1971) and is a generalization of the famous theorem of Elfving (1952) for scalar optimality. It 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

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

[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  $\varepsilon_1, \dots, \varepsilon_m \in \mathbb{R}^k$  with Euclidean norm 1 such that the point*

$$(2.3) \quad \gamma A = \sum_{i=1}^m p_i f(x_i)\varepsilon'_i$$

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  $\gamma A$  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)  $\text{tr}(\gamma A' D) = 1,$
- (ii)  $\|D' f(x)\|_2^2 = f'(x) D D' f(x) \leq 1$  for all  $x \in \mathcal{X}$

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

For our later investigations it is useful to identify the supporting hyperplane of the boundary point  $\gamma A$  in (2.3) of Theorem 2.3. It follows from the proof of this theorem [see Studden (1971)] that

$$(2.4) \quad \gamma A = M(\xi_A) D,$$

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

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

for any generalized inverse of  $M(\xi_A)$ .

**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 denotes the minimum eigenvalue of the information matrix of the  $E$ -optimal design  $\xi_E$  and  $\lambda_{\min}(B)$  denotes the minimum eigenvalue of a matrix  $B$ . By Theorem 2.1 the design  $\xi_E$  is  $E$ -optimal if and only if there exists a matrix  $E$  which satisfies (2.1) and has the representation

$$(3.1) \quad E = \sum_{i=1}^{k_0} \alpha_i z_i z_i',$$

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

LEMMA 3.1. Let  $\xi_E$  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  $z_1, \dots, z_{k_0}$  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 nonnegative definite matrix  $E$  (note that

$\rho_1, \dots, \rho_{k_0}$  are linearly independent). Let  $x$  denote a vector with  $z'_i x = 0$ ,  $i = 1, \dots, k$ . 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  $\text{nullspace}\{z_1, \dots, z_k\} \subseteq \text{nullspace}\{\rho_1, \dots, \rho_{k_0}\}$  or equivalently  $\text{span}\{\rho_1, \dots, \rho_{k_0}\} \subseteq \text{span}\{z_1, \dots, z_k\}$ . This shows that  $\rho_1, \dots, \rho_{k_0}$  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

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

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  $M(\xi_E)$  corresponding to the minimum eigenvalue  $\lambda_{\min}$ .  $\square$

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

**THEOREM 3.2.** *Let  $\xi_E$  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  $\xi_E$  is optimal for  $A'\theta$ , where  $A = (\sqrt{\alpha_1} z_1, \dots, \sqrt{\alpha_{k_0}} z_{k_0}) \in \mathbb{R}^{n \times k_0}$ .*

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

$$\lambda_{\min} \geq f'(x) E f(x) = f'(x) \sum_{i=1}^{k_0} (\sqrt{\alpha_i} z_i) (\sqrt{\alpha_i} z_i)' f(x) = \text{tr}(f'(x) A A' f(x)),$$

where  $A = (\sqrt{\alpha_1} z_1, \dots, \sqrt{\alpha_{k_0}} z_{k_0}) \in \mathbb{R}^{n \times k_0}$  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  $M(\xi_E) z_i = \lambda_{\min} z_i$ ]

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

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

$$\begin{aligned} \text{tr}(A' M^{-1}(\xi_E) f(x) f'(x) M^{-1}(\xi_E) A) &\leq \frac{1}{\lambda_{\min}} = \sum_{i=1}^{k_0} \alpha_i z'_i M^{-1}(\xi_E) z_i \\ &= \sum_{i=1}^{k_0} \alpha_i \text{tr}(M^{-1}(\xi_E) z_i z'_i) \\ &= \text{tr}(M^{-1}(\xi_E) A A') \end{aligned}$$

and it follows from Theorem 2.2 that the design  $\xi_E$  is optimal for  $A'\theta$ , where the matrix  $A$  is given by  $A = (\sqrt{\alpha_1}z_1, \dots, \sqrt{\alpha_{k_0}}z_{k_0})$ .  $\square$

REMARK. Reversing the above steps one can easily obtain a converse to Theorem 3.2. That is, suppose that the design  $\xi_A$  is optimal for  $A'\theta$ , where  $A = (\sqrt{\alpha_1}z_1, \dots, \sqrt{\alpha_{k_0}}z_{k_0})$  for some set  $\{\alpha_i\}_{i=1}^{k_0}$ ,  $\sum_{i=1}^{k_0}\alpha_i = 1$ , and  $z_1, \dots, z_{k_0}$  are linearly independent normalized eigenvectors corresponding to  $\lambda_{\min}(M(\xi_A)) > 0$ . Then the design  $\xi_A$  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 preceding 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  $\varepsilon'_1, \dots, \varepsilon'_m$  such that for the  $E$ -optimal design  $\xi = \left\{ \begin{matrix} x_i \\ p_i \end{matrix} \right\}_{i=1}^m$  the point

$$(3.2) \quad \gamma A = \sum_{i=1}^m p_i f(x_i) \varepsilon'_i$$

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  $A = (\sqrt{\alpha_1}z_1, \dots, \sqrt{\alpha_{k_0}}z_{k_0}) \in \mathbb{R}^{n \times k_0}$  is the matrix of Theorem 3.2. Moreover we have for the number  $\gamma$  from (2.5)

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

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

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

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 in-ball 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  $\xi_E$  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  $A_k = (\sqrt{\alpha_1}z_1, \dots, \sqrt{\alpha_{k_0}}z_{k_0}, 0, \dots, 0) \in \mathbb{R}^{n \times k}$ ,  $k_0 \leq k \leq n$ , where the last  $k - k_0$  columns of  $A_k$  contain only zeros. Then the

point  $\sqrt{\lambda_{\min}}A_k$  is an in-ball 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  $D_k = (D, 0, \dots, 0) \in \mathbb{R}^{n \times k}$  for any  $k \geq k_0$ . For the norm of  $A_k$  we obtain  $\|A_k\|_2^2 = \text{tr}(A_k A_k') = \sum_{i=1}^{k_0} \alpha_i z_i' z_i = 1$  which implies  $(\sqrt{\lambda_{\min}}A_k \in \partial \mathcal{R}_k)$

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

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  $\text{tr}(D'M(\xi)D) \leq 1$  for every design  $\xi$  on  $\mathcal{X}$ . This implies that

$$\begin{aligned} \frac{1}{\lambda_{\min}} &= \inf_{\xi} \sup_F \frac{\text{tr}(M^{-1}(\xi)FF')}{\text{tr}FF'} = \inf_{\xi} \sup_F \sup_G \left\{ \frac{\text{tr}^2(G'F)}{\text{tr}(G'M(\xi)G)} \frac{1}{\text{tr}(FF')} \right\} \\ &\geq \inf_{\xi} \sup_F \frac{\text{tr}^2(D'F)}{\text{tr}(D'M(\xi)D)} \frac{1}{\text{tr}(FF')} \geq \sup_F \frac{\text{tr}^2(D'F)}{\text{tr}(FF')} = \text{tr}(D'D). \end{aligned}$$

Here we have used the identity  $\text{tr}(M^{-1}FF') = \sup_G (\text{tr}^2 G'F / \text{tr}(G'MG))$  [see Studden (1971), page 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  $1/\text{tr}(D'D)$  we obtain for the squared in-ball radius the representation

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

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

Theorem 3.3 can roughly be summarized in the following way. Considering the Elfving sets  $\mathcal{R}_1, \mathcal{R}_2, \mathcal{R}_3, \dots$  there exists a number  $k_0$  such that all squared in-ball radii  $r_k^2$  are equal to the minimum eigenvalue of the  $E$ -optimal design for  $k \geq k_0$ . In every set  $\mathcal{R}_k$ ,  $k \geq k_0$ , there exists at least one in-ball 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  $z_1, \dots, z_{k_0}$  in the representation (3.1) we obtain that  $k_0 \leq n$ . This suggests the following procedure for the determination of  $E$ -optimal designs. Look at the in-ball vectors  $A$  of the set  $\mathcal{R}_n$  (because we do not know the numbers  $k_0 \leq n$  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  $n = 2$ ,  $f(x) = (x_1, x_2)$ ,  $\mathcal{X} = \left\{ \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \begin{pmatrix} 1/2 \\ 1 \end{pmatrix}, \begin{pmatrix} -1/2 \\ 1 \end{pmatrix} \right\}$ . 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 in-ball 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  $\begin{pmatrix} 1/2 \\ 1 \end{pmatrix}$  and  $\begin{pmatrix} -1/2 \\ 1 \end{pmatrix}$  is optimal for  $A'\theta$ , where  $A$  is an in-ball vector of  $\mathcal{R}_2$ . Its information matrix and its minimum eigenvalue are given by

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

and therefore the design  $\xi_A$  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  $\xi_E$  which puts equal mass at  $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$  and  $\begin{pmatrix} -1 \\ -1 \end{pmatrix}$  is also optimal for  $A'\theta$ . It is easily verified that this design is an  $E$ -optimal one.

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

THEOREM 3.4. *Let  $\xi_E$  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  $z_1, \dots, z_{k_0}$ . Whenever  $n \geq k \geq k_0$  and  $\sqrt{\lambda_{\min}}A$  is any in-ball 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 in-ball vector of  $\mathcal{R}_k$  and  $k \geq k_0$  we have from Theorem 3.3

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

which implies  $\text{tr}AA' = 1$ . Let  $\xi_A$  denote an optimal design for  $A'\theta$ . Then from



(Elfving's) Theorem 2.3 and (2.5) we obtain  $\lambda_{\min}^{-1} = \text{tr}(A'M^{-1}(\xi_A)A) = \inf_{\xi} \text{tr}(A'M^{-1}(\xi)A)$ . On the other hand, it follows for the  $E$ -optimal design  $\xi_E$  that

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

which shows that  $\xi_E$  is also optimal for  $A'\theta$  [because  $\text{tr}(A'M^{-1}(\xi_E)A)$  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  $\text{tr}(D'M(\xi)D) \leq 1$  for any design  $\xi$  on  $\mathcal{X}$  and we obtain

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

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

The results derived so far suggest the following procedure for the determination of the  $E$ -optimal design. First the in-ball radius of  $\mathcal{R}_n$ , an in-ball 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 in-ball 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 in-ball 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 in-ball 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

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

We will demonstrate this procedure in some examples in Section 4. The main step is the determination of the in-ball radius of  $\mathcal{R}_n$ . The following result gives estimates of the in-ball radius  $r_m$  by the in-ball radius  $r_k$ ,  $m \leq k$ , and is often very useful for the calculation of the in-ball radii of  $\mathcal{R}_k$ .

**THEOREM 3.5.** *Let  $r_k$  denote the in-ball radius of  $\mathcal{R}_k$ ,  $k = 1, \dots, n$ , 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 in-ball 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

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

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

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

From this inequality we obtain

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

which proves part (c) of the theorem.  $\square$

We should mention at this point that the bounds of (b) and (c) are sharp. More precisely, Example 2 in Section 4 provides situations for which  $\lambda_{\min}$  has multiplicity  $n$  and we have equality in (b) or (c).

Although the calculation of the in-ball 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  $\text{Eff}(\xi)$  of a design  $\xi$  from Theorem 3.5(b)

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

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 in-ball radii  $(r_1, r_2, \dots, r_n)$ .

**COROLLARY 3.6.** *Let  $r_k$  denote the in-ball radius of  $\mathcal{R}_k$  and  $f = \max\{i | r_i < r_{i-1}\}$  (if  $r_1 = r_2 = \dots = r_n$  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  $r_{k_0} = r_{k_0+1} = \dots = r_n$  which implies  $f \leq k_0 \leq$  multiplicity of  $\lambda_{\min}$ .  $\square$

**4. Examples.**

**4.1. Spring balance weighing designs.** In a recent paper Cheng (1987) investigated  $\Phi_p$ -optimal designs for the regression setup  $f(x) = x = (x_1, x_2, \dots, x_n)$ ,  $\mathcal{X} = \{0, 1\}^n$  (Cheng considers  $\chi = [0, 1]^n$ ; however, these are equivalent in the ‘‘approximate’’ theory). 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  $\Phi_p$ -optimal approximate designs. For  $p = \infty$  he found the  $E$ -optimal spring balance weighing design. By the application of our results we can present a 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 in-ball radius (here the index  $n$  represents the number of regression functions). Let  $D' = (d_1, \dots, d_n) \in \mathbb{R}^{k \times n}$  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  $d_1, \dots, d_n$  denote here the columns of  $D'$ ). For the determination of the in-ball radius  $r_k(n)$  of  $\mathcal{R}_k^n$ ,  $k \leq n$ , we have to solve the problem [see (3.6)]

$$(4.1) \quad \text{Minimize } \frac{1}{\text{tr}(DD')} \quad \text{subject to } \|D'x\|_2 \leq 1 \quad \forall x \in \mathcal{X}.$$

Inserting all possible points  $x \in \mathcal{X} = \{0, 1\}^n$  in the constraint, (4.1) is equivalent to the problem

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

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

$$(4.2) \quad \sum_{i \in I} \|d_i\|_2^2 + \sum_{\substack{i \in I \\ j \in I \\ i \neq j}} d'_i d'_j = \left\| \sum_{i \in I} d_i \right\|_2^2 \leq 1$$

for all subsets  $I \subseteq \{1, \dots, 2m\}$ . Considering only the subsets  $I$  with exactly  $m$  elements and adding the inequalities of (4.2) corresponding to these sets we obtain

$$(4.3) \quad \binom{2m-1}{m-1} \sum_{i=1}^{2m} \|d_i\|_2^2 + \frac{\binom{2m}{m} \binom{m}{2}}{\binom{2m}{2}} \sum_{i=1}^{2m} \sum_{\substack{j=1 \\ j \neq i}}^{2m} d'_i d'_j \leq \binom{2m}{m}.$$

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 (4.3) reduces after some algebra to

$$(4.4) \quad \text{tr}(DD') = \sum_{i=1}^{2m} \|d_i\|_2^2 \leq \frac{2(2m-1)}{m}.$$

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

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

satisfies  $\|D'_0 x\|_2^2 \leq 1$  for all  $x \in \{0, 1\}^{2m}$  and that  $\text{tr} D_0 D'_0 = 2(2m-1)/m$ . This shows that  $D_0$  is a solution of the problem (4.1) and that the in-ball 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 in-ball vector of  $\mathcal{R}_{2m}^{2m}$  is given by  $\sqrt{\lambda_{\min}} A = (m/2(m-1))D_0$  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

$$\{x \mid \|D'_0 x\|_2 = 1\} = \{x \in \{0, 1\}^{2m} \mid x \text{ has exactly } m \text{ components equal } 1\}.$$

Let  $\{v_i\}$  denote the set of vectors in  $\mathbb{R}^{2m}$  with  $m$  components 0 and  $m$  components 1, then it is straightforward to show that the design  $\xi_E$  which

puts uniform mass on the  $\binom{2m}{m}$  vectors  $v_i$  has information matrix  $M(\xi_E) = (m/2(2m - 1))I_{2m} + ((m - 1)/2(2m - 1))J_{2m}$  with minimum eigenvalue  $\lambda_{\min} = m/2(2m - 1)$  (here  $I_{2m}$  denotes the identity matrix and  $J_{2m}$  the matrix with all elements equal 1). Therefore  $\xi_E$  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  $r_{2m+1}^2(2m + 1) = \lambda_{\min} = (m + 1)/2(2m + 1)$  and has multiplicity  $2m$ .

For the determination of  $E$ -optimal design it is sufficient to look at the set  $\mathcal{R}_n^n$  and its corresponding in-ball radius  $r_n(n)$ . However for the illustration of the theorems of Section 3 it might be useful to investigate also the in-ball radius  $r_k(n)$  for  $k < n$  in this example. At first we will show that the in-ball 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 (4.4) does not depend on the dimension of the vectors  $d_i$  we still have  $r_{2m-1}^2(2m) \geq m/2(2m - 1)$ . Let  $\tilde{D}_0 = (\tilde{d}_1, \dots, \tilde{d}_{2m-1}) \in \mathbb{R}^{2m \times (2m-1)}$ , where

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

$i = 1, \dots, 2m - 1$ . Then it is straightforward to check that  $\tilde{D}_0$  fulfills  $\|\tilde{D}'_0 x\|_2 \leq 1$  for all  $x \in \mathcal{X}$  and  $\text{tr}(\tilde{D}_0 \tilde{D}'_0) = 2(2m - 1)/m$ . 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  $r_k(n) \leq r_k(k + 1)$  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  $r_{2m+1}^2(2m + 2) = r_{2m+2}^2(2m + 2) = (m + 1)/2(2m + 1) = r_{2m+1}^2(2m + 1)$ . 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  $\|D'x\|_2 \leq 1 \forall x \in \{0, 1\}^{2m+3}$ . 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  $90^\circ$ . Therefore  $D'$  contains at least two vectors, say  $d_1$  and  $d_2$  with  $d'_1 d_2 \geq 0$ . 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  $\|\tilde{D}'x\|_2 \leq 1$  (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  $\text{tr} \tilde{D}' \tilde{D}' \geq \text{tr} D' D'$ . 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  $r_{2m+1}^2(2m + 2)$  and we have from (3.6)

$$r_{2m+1}^2(2m + 2) \leq \frac{1}{\text{tr}(D'_0 D_0)} = \frac{1}{\text{tr}(\tilde{D}' \tilde{D}')} \leq \frac{1}{\text{tr}(D' D')}$$

TABLE 1

The squared in-ball radii of the sets  $\mathcal{D}_k^n$  ( $n \leq 7, k \leq 7$ ) for the spring balance weighing designs

k	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	...
	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

for all matrices  $D \in \mathbb{R}^{(2m+3) \times (2m+1)}$  satisfying  $\|D'x\|_2 \leq 1, x \in \{0, 1\}^{2m+3}$ . This shows  $r_{2m+1}(2m + 2) \leq r_{2m+1}(2m + 3)$  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  $r_{2m+1}(n) = r_{2m+1}(2m + 1)$  for all  $n \geq 2m + 1$ . For the case  $k = 2m$  we apply Theorem 3.5(a) and obtain by similar arguments  $r_{2m}(n) = r_{2m}(2m + 1)$  whenever  $n \geq 2m + 1$ . Summarizing all results obtained so far we have for the squared in-ball radii  $r_k^2(n)$  in the spring balance weighing design example,

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

The squared in-ball radii are illustrated in Table 1 for  $n \leq 7, k \leq 7$ .

We see that for fixed  $n$  the sequence of in-ball radii  $(r_1, r_2, r_3, \dots)$  is not strictly decreasing.

4.2. *Linear 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 example. Only some special cases—for example,  $p = 2$  or  $p = \infty$  (chemical balance weighing designs)—arise in various applications of linear regression. Let  $f(x) = x = (x_1, \dots, x_n)$ , the design space is  $\mathcal{X} = \{x \mid \|x\|_p \leq 1\}$ , where  $\|x\|_p = (\sum_{i=1}^n |x_i|^p)^{1/p}$  denotes the  $l_p$ -norm on  $\mathbb{R}^n, 1 \leq p \leq \infty$ . 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  $D' = (d_1, \dots, d_n) \in \mathbb{R}^{n \times n}$  such that  $\|D'x\|_2 \leq 1$  for all  $x \in \mathcal{X}$ . Inserting the unit vectors  $e_i = (0, \dots, 0, 1, 0, \dots, 0)' \in \mathbb{R}^n$  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) in-ball vector  $r_n^2(n)$ , that is,  $r_n^2(n) \geq 1/n$ . For the matrix  $D = I_n$  we have (note that  $p \leq 2$ )  $\|Dx\|_2 = \|x\|_2 \leq \|x\|_p \leq 1$  and  $\text{tr}(D'D) = 1/n$ , which shows that  $r_n^2(n) = 1/n$ . From Theorems 3.3 and 3.4 we conclude that  $\lambda_{\min} = 1/n$  and by straightfor-

ward arguments it can be shown that the  $E$ -optimal design puts equal masses at the points  $e_i, i = 1, \dots, n$ .

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

$$2^{n-1}n^{-2/p} \sum_{i=1}^n d'_i d_i \leq 2^{n-1},$$

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  $\text{tr}(DD') = n^{2/p}$ . 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  $(1/p + 1/q = 1)$

$$\begin{aligned} \|D'_0x\|_2^2 &= n^{2/p-1}\|x\|_2^2 = n^{2/p-1} \sum_{i=1}^n x_i^2 \\ &\leq n^{2/p-1} \left( \sum_{i=1}^n |x_i|^p \right)^{1/p} \left( \sum_{i=1}^n |x_i|^q \right)^{1/q} \leq \|x\|_p^2 \leq 1 \end{aligned}$$

that  $D_0$  satisfies also the other condition. Here we have used the inequality  $n^{2/p-1}\|x\|_q \leq \|x\|_p$  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  $n^{-1/p}(\mp 1, \mp 1, \dots, \mp 1)$  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  $\|D'_0x\|_2 = 1$  of Theorem 3.4 reduces to  $\|x\|_2 = 1$ . For example, the design which puts equal masses at the unit vectors  $e_i$  is also  $E$ -optimal. Note also that the case  $p = \infty$  yields to the  $E$ -optimal chemical weighing designs.

4.3. *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 in-ball radii of the first two Elfving sets  $\mathcal{R}_1$  and  $\mathcal{R}_2$ . Let  $d = (0, -3/b, 0, 4/b^3)'$  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)]

$$(4.5) \quad \lambda_{\min} \leq r_1^2 \leq \left[ \left( \frac{3}{b} \right) + \left( \frac{4}{b^3} \right)^2 \right]^{-1}.$$

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  $\mp \sqrt{(1-\alpha)/2(2-\alpha)}b$  and that this maximum is equal 1). Therefore we have

$$(4.6) \quad \frac{1}{r_2^2} \geq g(\alpha) := \text{tr}(DD') = \alpha(2-\alpha) \left( 1 + \frac{4}{b^4} \right) + \frac{(3-\alpha)^2}{b^2} + \frac{4(2-\alpha)^2}{b^6}$$

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  $f''(\alpha) = -(2/b^6)(b^2 - 1)(b^4 + 4) < 0$  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 (4.6) we



obtain the upper bound

$$(4.7) \quad \lambda_{\min} \leq r_2^2 \leq \begin{cases} \frac{b^2(b^2 - 1)(b^4 + 4)}{b^8 + 3b^6 + 8b^4 + 12b^2 + 12}, & \text{if } b \geq b_0, \\ \left[ \left( \frac{3}{b} \right)^2 + \left( \frac{4}{b^3} \right)^2 \right]^{-1}, & \text{if } b \leq b_0. \end{cases}$$

Because  $f(\alpha_{\max}) > f(0) = (3/b)^2 + (4/b^3)^2$  whenever  $b > b_0$ , we see from (4.7) that for  $b > b_0$  the minimum eigenvalue of the  $E$ -optimal design is *not* given by  $\|d\|_2^{-2}$ , where  $d = (0, -3/b, 0, 4/b^3)$  denotes the vector of the coefficients of the third Chebyshev polynomial on  $[-b, b]$  [ $d'f(x) = T_3(x/b)$ ]. The same arguments will hold for polynomial regression of arbitrary degree  $n \geq 2$  on  $[-b, b]$ .

The calculation of the in-ball 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 in-ball radii  $r_k$  are very useful for the calculation of  $E$ -efficiencies for a given design. As an illustration we consider the case  $b = 3$  and obtain from (4.7)  $\lambda_{\min} \leq r_2^2 \leq 510/793 = 0.6431$ , which gives the lower bound for the  $E$ -efficiency of a given design  $\xi$  [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  $\eta$  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  $\text{Eff}(\eta) \geq 91.44\%$ . If we put masses proportional to 1:9:9:1 at the same points, we obtain a minimum eigenvalue 0.6137 and an  $E$ -efficiency greater than or equal to 94.42%.

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