The Annals of Statistics
1994, Vol. 22, No. 2, 917–929

E-OPTIMAL DESIGNS IN WEIGHTED POLYNOMIAL REGRESSION

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Based on a duality between E-optimality for (sub-) parameters in weighted polynomial regression and a nonlinear approximation problem of Chebyshev type, in many cases the optimal approximate designs on nonnegative and nonpositive experimental regions $[a, b]$ are found to be supported by the extrema of the only equioscillating weighted polynomial over this region with leading coefficient 1. A similar result is stated for regression on symmetric regions $[-b, b]$ for certain subparameters, provided the region is "small enough," for example, $b \leq 1$. In particular, by specializing the weight function, we obtain results of Pukelsheim and Studden and of Dette.

1. Introduction. Consider polynomial regression of degree $d \geq 1$,

$$y(x) = \sum_{i=0}^{d} \vartheta_i x^i, \qquad x \in [a, b],$$

where the controlled variable x is chosen from the interval $[a, b]$ and $\theta = (\vartheta_0, \dots, \vartheta_d)'$ (the prime denotes transposition) is an unknown parameter vector. This setup is embedded in the usual statistical context: for estimating θ (or a subvector $K\theta$ of θ), uncorrelated random variables Y_{x_ν} can be observed under experimental conditions $x_\nu \in [a, b]$, such that Y_{x_ν} has expectation $y(x_\nu)$ and variance $\sigma^2/\omega(x_\nu)$, $1 \leq \nu \leq n$, where $\sigma^2 > 0$ and $\omega \not\equiv 0$ is some nonnegative and continuous weight function (also called efficiency function) on $[a, b]$.

A design ξ is a probability measure on $[a, b]$ with finite support. The weights of ξ give the ideal proportions of observations to be taken under the experimental conditions designated by its support. Let $M(\xi) = (m_{\mu+\nu}(\xi))_{0 \leq \mu, \nu \leq d}$ denote the moment matrix of ξ, built in the (weighted) moments $m_\mu(\xi) = \int \omega(x) x^\mu \, d\xi(x)$, $\mu \leq 2d$. The choice of a design ξ is based on its information matrix $C_K(M(\xi))$ for $K\theta$,

$$C_K(M(\xi)) = \min\{LM(\xi)L' : L \in \mathcal{G}_{K'}\},$$

where the minimum refers to the Löwner partial ordering, and $\mathcal{G}_{K'}$ is the set of g-inverses of K' [see, e.g., Gaffke (1987)]. A design is called E-optimal design for $K\theta$ if it maximizes the smallest eigenvalue $\lambda_{\min}[C_K(M(\xi))]$ of the information matrices for $K\theta$ among all designs.

Received August 1992; revised October 1993.
AMS 1991 *subject classification.* 62K05.
Key words and phrases. Approximate designs, E-optimal designs, Chebyshev approximation, Chebyshev system, total positivity, weighted polynomial regression.

In the case of $\omega \equiv 1$ and $[a,b] = [-1,1]$, the E-optimal design problem is partially solved in Pukelsheim and Studden (1993); see also Dette and Studden (1993). Based on a duality between E- and c-optimality [A-optimality in Dette and Studden (1993)], the optimal design for certain subparameters is found to be supported by the extreme points of the Chebyshev polynomial of the first kind of degree d, as conjectured by Preitschopf (1989), and an explicit formula for its weights is given. E-optimal designs in case $\omega(x) = (1+x)^{\alpha}(1-x)^{\beta}$, $x \in [a,b] = [-1,1]$, with $\alpha, \beta \in \{0,1\}$ are shown in Dette (1993) to be supported by the zeros of certain weighted Jacobi polynomials.

We utilize here another aspect of the duality to E-optimality. In Section 2 we obtain from general equivalence theorems for optimal designs that the E-optimal design ξ_0 is supported by the extreme points of a solution to a nonlinear Chebyshev approximation problem. Section 3 gives conditions under which ξ_0 can be computed explicitly: if $[a,b]$ is nonnegative (or nonpositive) and if there exists a solution to the nonlinear approximation problem with (at most) $d+1$ global maxima in $[a,b]$, then, unless $a = 0$ and $K\theta = \vartheta_0$, ξ_0 is supported by the $d+1$ extrema of the *only* equioscillating polynomial built in $\sqrt{\omega(x)}x^{\mu}$, $0 \le \mu \le d$, with leading coefficient 1, and a formula for the associated weights is verified.

A main step for obtaining this description of ξ_0 is to identify a solution to the nonlinear approximation problem as square of a polynomial in $\sqrt{\omega(x)}x^{\mu}$, $0 \le \mu \le d$, with coefficients given by the coordinates of an eigenvector of $C_K(M(\xi_0))$ to $\lambda_{\min}[C_K(M(\xi_0))]$. Here, the results in Heiligers (1994) imply that $C_K(M(\xi_0))$ is totally positive (up to multiplication of certain rows and columns by -1), a property which entails simplicity of the smallest eigenvalue and a characteristic sign pattern of the coordinates of the corresponding eigenvector.

Similar characterizations of optimal designs for *certain* subparameters $K\theta$ hold true if the experimental region and the weight function are symmetric around zero, provided the region is not "too large." Then $C_K(M(\xi_0))$ decomposes into a principal block diagonal matrix with two diagonal blocks, both of which possess a simple smallest eigenvalue. These values can be compared successfully if the region is "small enough" and if the system of parameters of interest satisfies the "neighborhood" condition from Pukelsheim and Studden (1993).

2. E-optimality and Chebyshev approximation. We denote by $f(x) = (1, x, \dots, x^d)'$, $x \in \mathbb{R}$, the vector of monomials in x up to degree d. Let $\mathcal{I} \subseteq \{0, \dots, d\}$ describe the (s-dimensional) subparameter of interest, that is, $K\theta = (\vartheta_i)_{i \in \mathcal{I}}$, and let $\mathcal{P}_{K'}$ be the set of nonnegative (weighted) polynomials $p_{Z,L} = \omega f'L'ZLf$, where L ranges over $\mathcal{G}_{K'}$ and Z ranges over the set of nonnegative definite $s \times s$ matrices with trace$[Z] = 1$. Consider the approximation problem of Chebyshev type,

$$\text{(1)} \qquad \text{minimize} \quad \max_{x \in [a,b]} p_{Z,L}(x) \quad \text{over } p_{Z,L} \in \mathcal{P}_{K'}.$$

The following duality between E-optimality and problem (1) can be deduced from the general equivalence theorems developed in convex design theory; see, for example Pukelsheim (1980) and Gaffke (1987) [cf. Heiligers (1992), Lemma

(2.4)]. Note that these equivalence theorems also ensure the existence of a solution to (1).

We denote by $\mathcal{E}(p)$ the set of global maxima of the polynomial $p \in \mathcal{P}_{K'}$ in $[a, b]$ and by supp(ξ) the support of the design ξ.

THEOREM 1. *Let ξ be a design and $p_{Z,L}$ be a polynomial from $\mathcal{P}_{K'}$. Then*

$$\lambda_{\min}\Big[C_K\big(M(\xi)\big)\Big] \le \max_{x \in [a,b]} p_{Z,L}(x),$$

with equality for $\xi = \xi_0$ and $p_{Z,L} = p_{Z_0,L_0}$ iff ξ_0 is E-optimal for $K\theta$ and p_{Z_0,L_0} solves (1), *equivalently, iff the following three conditions are fulfilled*:

(i) $L_0 M(\xi_0) L_0' Z_0 = C_K(M(\xi_0)) Z_0 = (\max_{x \in [a,b]} p_{Z_0,L_0}(x)) Z_0$;
(ii) $\max_{x \in [a,b]} p_{Z_0,L_0}(x) = \lambda_{\min}[C_K(M(\xi_0))]$;
(iii) $\operatorname{supp}(\xi_0) \subseteq \mathcal{E}(p_{Z_0,L_0})$.

The duality stated above is closely related to the approach to E-optimality considered in Dette and Studden (1993): It can be shown that if p_{Z_0,L_0} solves (1), then the matrix $V_0 \in \mathbb{R}^{s \times r}$ chosen from a full-rank factorization $Z_0 = V_0 V_0', \operatorname{rank}(Z_0) = r$, defines an in-ball vector of the generalized Elfving set $\operatorname{conv}(\{\sqrt{\omega(x)} L_0 f(x) \varepsilon' : x \in [a,b], \varepsilon \in \mathbb{R}^r, \|\varepsilon\| = 1\}), \|\varepsilon\|^2 = \varepsilon'\varepsilon$ [cf. Heiligers (1992), page 28].

According to Theorem 1, an E-optimal design ξ_0 for $K\theta$ can be computed as follows. If we can find a solution p_0 to (1) with finitely many global maxima in $[a, b]$, then ξ_0 is supported by $\mathcal{E}(p_0)$ with weights solving the system of linear equations associated with condition (i) from above. Actually, if p_0 has *at most* $d + 1$ global maxima in $[a, b]$, then these equations have a unique solution. [It should be noted that the particular formula for the weights of an optimal design stated below becomes important in Section 3. This formula is also obtainable from the results in Pukelsheim and Torsney (1991) or Dette and Studden (1993); this, however, requires roughly the same arguments as in the present proof.]

THEOREM 2. *Let $p_0 = p_{Z_0,L_0} \in \mathcal{P}_{K'}$ be a solution to* (1) *with at most $d + 1$ global maxima in $[a, b]$ [$\mathcal{E}(p_0) = \{x_0, \dots, x_t\}$, $t \le d$, say]. Then the E-optimal design ξ_0 for $K\theta$ is uniquely determined; ξ_0 is concentrated on $\mathcal{E}(p_0)$, and the weights can be obtained as follows.*

*Set $F = (x_\nu^\mu)_{0 \le \mu \le d, 0 \le \nu \le t}$ and represent $Z_0 = \sum_{j=1}^{\ell} \beta_j z_j z_j'$ (where $\beta_j > 0$, $\sum_{j=1}^{\ell} \beta_j = 1$, $z_j' z_j = 1$) as a convex combination of rank-*1 *matrices $z_j z_j'$. Let $e_\nu, 0 \le \nu \le t$, denote the unit vectors in $\mathbb{R}^{t+1}$, and define*

$$\Delta_\nu = \frac{e_\nu'(F'F)^{-1} F' K' z_{j_\nu}}{\omega(x_\nu) f'(x_\nu) L_0' z_{j_\nu}}, \quad 0 \le \nu \le t,$$

where, for each $0 \le \nu \le t, j_\nu \in \{1, \dots, \ell\}$ is arbitrary with $\omega(x_\nu) f'(x_\nu) L_0' z_{j_\nu} \ne 0$. Then

$$\xi_0(x_\nu) = \frac{\Delta_\nu}{\sum_{\mu=0}^{t} \Delta_\mu} \quad \text{for all } 0 \le \nu \le t.$$

PROOF. Let ξ_0 be E-optimal for $K\theta, M_0 = M(\xi_0)$. Set $P_0 = I_{d+1} - K'L_0$. Observing that $\mathcal{G}_{K'} = \{L_0 + DP_0 \colon D \in \mathbb{R}^{s \times (d+1)}\}$, it follows from Theorem 1 that

$$\begin{aligned} 0 &\leq \operatorname{trace}\left[(L_0 + \kappa DP_0)M_0(L_0 + \kappa DP_0)'Z_0\right] - \operatorname{trace}\left[L_0 M_0 L_0' Z_0\right] \\ &= \kappa^2 \operatorname{trace}\left[DP_0 M_0 P_0' D' Z_0\right] + 2\kappa \operatorname{trace}\left[DP_0 M_0 L_0' Z_0\right] \quad \text{for all } \kappa \in \mathbb{R}; \end{aligned}$$

thus $\operatorname{trace}[DP_0 M_0 L_0' Z_0] = 0$ for all $D \in \mathbb{R}^{s \times (d+1)}$, and $P_0 M_0 L_0' Z_0 = 0$, that is,

$$M_0 L_0' z_j = K' L_0 M_0 L_0' z_j \quad \text{for all } 1 \leq j \leq \ell.$$

Moreover, by Theorem 1, the z_j are normalized eigenvectors of $L_0 M_0 L_0'$ to the smallest eigenvalue $\lambda_0 = \lambda_{\min}[C_K(M_0)]$, and therefore (for all $1 \leq j \leq \ell$ and all $0 \leq \nu \leq t$)

$$\xi_0(x_\nu)\omega(x_\nu)f'(x_\nu)L_0' z_j = \lambda_0 e_\nu'(F'F)^{-1}F'K'z_j. \tag{2}$$

For each $0 \leq \nu \leq t$ there exists a $1 \leq j_\nu \leq \ell$ such that $\omega(x_\nu)f'(x_\nu)L_0' z_{j_\nu} \neq 0$; otherwise, $\omega(x_\nu)f'(x_\nu)L_0' z_j = 0$ for all $1 \leq j \leq \ell$ and some $0 \leq \nu \leq t$. Thus $p_0(x_\nu) = \sum_{j=1}^{\ell} \beta_j \omega(x_\nu)(f'(x_\nu)L_0' z_j)^2 = 0$ and $p_0 \equiv 0$, contrary to our assumption. Now the assertion follows from (2), since the weights of ξ_0 sum up to 1. □

We state here two examples for setups such that there exists a solution to (1) with at most $d+1$ global maxima in $[a,b]$. The proof of Lemma 3 can be found in Heiligers [(1992), page 35ff.]; the proof of Lemma 4 is as that of Theorem 7.4 in Karlin and Studden (1966).

LEMMA 3. *Let* $\omega \equiv 1$. *Then there exists a solution to* (1) *with at most* $d+1$ *global maxima in* $[a,b]$ *iff (at least) one of the following four conditions is fulfilled*:

(i) $0 \notin \mathcal{J}$;
(ii) $d \geq 2$;
(iii) $d = 1, \mathcal{J} = \{0, 1\}$ *and* $-ab \leq 1$;
(iv) $d = 1, \mathcal{J} = \{0\}$ *and* $0 \notin (a,b)$.

LEMMA 4. *In each of the following cases, all solutions to* (1) *have at most* $d+1$ *global maxima in* $[a,b]$:

(i) $\omega(x) = (x - a_1)^\alpha (b_1 - x)^\beta$, $x \in [a,b]$, *with* $a_1 \leq a < b \leq b_1$ *and* $\alpha, \beta > 0$;
(ii) $\omega(x) = \exp\{-x\}x^\alpha$, $x \in [a,b]$, *where* $a \geq 0$ *and* $\alpha \geq 0$;
(iii) $\omega(x) = \exp\{-x^2\}$, $x \in [a,b]$;
(iv) $\{1, \omega(x), \omega(x)x, \dots, \omega(x)x^{2d}\}$ *is a Chebyshev system over* $[a,b]$;
(v) ω^{-1} *is a positive polynomial on* $[a,b]$, *and the* $(2d+1)$*th derivative of* ω^{-1} *has no zeros in* (a,b);
(vi) ω *can be approximated uniformly by functions of the type considered in* (v).

A direct minimization of the Chebyshev norm of $p \in \mathcal{P}_{K'}$ over $[a,b]$ seems to be a difficult task. Even the problem of checking whether or not a given nonnegative polynomial belongs to $\mathcal{P}_{K'}$ is not trivial. To give an example, consider the case $K\theta = \theta$. By some small modifications in the proof of Lemma 3.2 in Heiligers (1988) it is seen that for each nonnegative weighted polynomial p there exists a nonnegative definite matrix V with $p = \omega f'Vf$. In general, however, if $d \geq 2$, then this matrix is not uniquely determined and even the trace of corresponding matrices can depend on the particular choice of V [see Heiligers (1992), page 29].

3. *E*-optimal designs. For characterizing E-optimality in Theorem 7, below, we have to ensure that an optimal design has *at least* $d+1$ support points. In this context it is helpful to find conditions implying that an arbitrary design ξ with regular information matrix for $K\theta$ possesses a regular moment matrix $M(\xi)$, that is,

$$\#\big(\operatorname{supp}(\xi) \cap \{x\colon \omega(x) \neq 0\}\big) \geq d+1. \tag{3}$$

The following lemma states results on this problem; slightly weaker statements are given in Preitschopf [(1989), Satz 2.9.4 and Satz 2.9.5].

LEMMA 5. *In both of the following cases, regularity of* $C_K(M(\xi))$ *is equivalent to* (3):

(i) ξ *has nonnegative* (*or nonpositive*) *support, and* $0 \notin \operatorname{supp}(\xi)$ *or* $\mathcal{I} \neq \{0\}$.

(ii) ξ *has symmetric support, that is,* $\operatorname{supp}(\xi) = \{x_0, \dots, x_t\} = \{-x_0, \dots, -x_t\}$, *and there is at least one integer* $i \in \mathcal{I}, i \neq 0$, *such that* $d - i$ *is even.*

PROOF. We show that under (i) or (ii) regularity of $C_K(M(\xi))$ implies (3); the converse implication holds triviality true. We consider case (i) only; case (ii) can be treated similarly.

Assume without loss of generality that ξ has nonnegative support. Suppose that ξ does not fulfil (3) (i.e., $\operatorname{supp}(\xi) \cap \{x\colon \omega(x) \neq 0\} = \{x_0, \dots, x_{t-1}\}, t \leq d$, say), but $C_K(M(\xi))$ is regular. Then, with $F = (x_\nu^\mu)_{0 \leq \mu \leq d, 0 \leq \nu \leq t-1}$, it follows from Krafft (1983) that

$$\operatorname{nullspace}\big(M(\xi)\big) = \operatorname{nullspace}(F') \subseteq \operatorname{nullspace}(K). \tag{4}$$

Choose positive numbers $x_t, \dots, x_{d-1}$ and consider the polynomial $q(x) = \Pi_{\nu=0}^{d-1} (x - x_\nu) = \Sigma_{\mu=0}^{d} a_\mu x^\mu$, $x \in \mathbb{R}$. For $\mu \geq 1$ the coefficients

$$a_\mu = (-1)^{d-\mu} \sum_{\substack{\mathcal{L} \subseteq \{0,\dots,d-1\} \\ \#\mathcal{L} = d-\mu}} \prod_{\ell \in \mathcal{L}} x_\ell$$

are different from zero, since at least $d-1$ of the x_ν's are positive. [If $0 \notin \operatorname{supp}(\xi)$, then also $a_0 \neq 0$]. Thus, $a = (a_0, \dots, a_d)' \in \operatorname{nullspace}(F')$, but $a \notin \operatorname{nullspace}(K)$, contrary to (4). $\square$

Some further remarks are helpful for investigating E-optimal designs in the case that the region $[a, b]$ and the weight function ω are symmetric around zero, that is, $a = -b$ and $\omega(x) = \omega(-x)$ for all $x \in [-b, b]$. Under these symmetries there exists an E-optimal design ξ_0 for $K\theta$, which is symmetric around zero, that is, such that $\xi_0(x) = \xi_0(-x)$ for all $x \in [-b, b]$.

Moment and information matrix of any symmetric design ξ decompose into principal block diagonal matrices with (at most) two diagonal blocks. Precisely, let the subvectors f_ℓ, $\ell = 1, 2$ of f (of dimension $d_\ell + 1$, say) consist of the monomials in x whose degrees differ from d by odd numbers if $\ell = 1$, and by even numbers if $\ell = 2$. Then, apart from suitable permutations of the rows and columns, $M(\xi) = \text{diag}(M_1(\xi), M_2(\xi))$, where $M_\ell(\xi) = \int \omega f_\ell f_\ell' \, d\xi$ is built in the moments of ξ of even degree [the moment $m_{2d}(\xi)$ of highest degree $2d$ is an entry of $M_2(\xi)$]. Obviously, $M_\ell(\xi)$ may be viewed as a $(d_\ell + 1) \times (d_\ell + 1)$-dimensional moment matrix of a certain design $\widehat{\xi}$ with nonnegative support, built w.r.t. ω_ℓ, where $\omega_1(x) = \omega(x)$ and $\omega_2(x) = x^2\omega(x)$ if d is odd, and $\omega_1(x) = x^2\omega(x)$ and $\omega_2(x) = \omega(x)$ if d is even.

Similarly, $C_K(M(\xi)) = \text{diag}(C_{K_1}(M_1(\xi)), C_{K_2}(M_2(\xi)))$, where, for $\ell = 1, 2$, $C_{K_\ell}(M_\ell(\xi))$ coincides with the information matrix of $\widehat{\xi}$ (considered as a design for polynomial regression $y_\ell(x) = \sum_{i=0}^{d_\ell} \vartheta_{i,\ell} x^i$, $x \in [0, b^2]$, of degree d_ℓ and weight function ω_ℓ) for the subparameters $K_\ell\theta_\ell = (\vartheta_{i,\ell})_{i \in \mathcal{J}_\ell}$, respectively with $\mathcal{J}_1 = \{d_1 - j : d - 2j - 1 \in \mathcal{J}\}$ and $\mathcal{J}_2 = \{d_2 - j : d - 2j \in \mathcal{J}\}$. [If $\mathcal{J}$ consists either of odd or of even integers only, then $C_K(M(\xi)) = C_{K_1}(M_1(\xi))$ or $C_K(M(\xi)) = C_{K_2}(M_2(\xi))$; in these cases the E-optimal design for $K\theta$ is easily obtained from the optimal design (in polynomial regression of degree d_1 and d_2 on $[0, b^2]$ and weight function ω_1 and ω_2) for $K_1\theta_1$ and $K_2\theta_2$, respectively]. If $\mathcal{J}$ contains even *and* odd integers and if $\mathcal{J}$ fulfills the "neighborhood" condition (5) considered in Pukelsheim and Studden (1993),

$$\text{(5)} \qquad \mathcal{J} \neq \{0\} \quad \text{and} \quad d - 2j - 1 \in \mathcal{J} \text{ implies } d - 2j \in \mathcal{J},$$

then the smallest eigenvalue of the complete information matrix $C_K(M(\xi))$ comes from the submatrix $C_{K_2}(M_2(\xi))$, at least if $b \leq 1$.

LEMMA 6. *Let $b \leq 1$ and suppose that $\mathcal{J}$ satisfies* (5). *Then we have, for all symmetric designs ξ,*

$$\lambda_{\min}\Big[C_{K_2}\big(M_2(\xi)\big)\Big] \leq \lambda_{\min}\Big[C_{K_1}\big(M_1(\xi)\big)\Big],$$

with strict inequality if $M(\xi)$ is regular and $b < 1$.

PROOF. We consider only the case $0 \in \mathcal{J}$ and $d = 2m$ even; all other cases are essentially the same.

For convenience, we rearrange the vectors f_ℓ and the columns of K_ℓ as follows. Let $\mathcal{J}_{1,1}$ and $\mathcal{J}_{1,2}$ be the sets of odd integers i with $i \in \mathcal{J}$, and $i \notin \mathcal{J}$ but $i + 1 \in \mathcal{J}$, respectively, and let $\mathcal{J}_{1,3}$ consist of the remaining odd integers from $\{1, \dots, d-1\}$. Set $f_{1,k}(x) = (x^i)_{i \in \mathcal{J}_{1,k}}$, $1 \leq k \leq 3$ (if some of the sets $\mathcal{J}_{1,k}$ are empty, the corresponding subvectors of f_1 are undefined), and arrange f_1 according to $f_1' = (f_{1,1}', f_{1,2}', f_{1,3}')$. Let $f_2' = (f_{2,1}', f_{2,2}', f_{2,3}', 1)$ and $f_{2,k}(x) = x f_{1,k}(x)$, $1 \leq k \leq 3$.

When arranging the columns of K_ℓ accordingly then, due to (5),

$$K_1 = (I_{s_1}, 0) \quad \text{and} \quad K_2 = \begin{pmatrix} I_{s_1} & 0 & 0 & 0 \\ 0 & I_{s_2-s_1-1} & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

where $s_\ell = \#\mathcal{J}_\ell, \ell = 1, 2$. Choose a g-inverse L_1 of K_1' with $C_{K_1}(M_1(\xi)) = L_1 M_1(\xi) L_1'$ and a normalized eigenvector z_1 of $C_{K_1}(M_1(\xi))$ to $\lambda_{\min}[C_{K_1}(M_1(\xi))]$. Partition $L_1 = (I_{s_1}, B_{1,2}, B_{1,3})$ according to f_1, and define the g-inverse L_2 of K_2' and the vector z_2 by

$$L_2 = \begin{pmatrix} I_{s_1} & 0 & B_{1,3} & 0 \\ 0 & I_{s_2-s_1-1} & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad z_2' = (z_1', z_1' B_{1,2}, 0').$$

[Note that $z_2' L_2 f_2(x) = x z_1' L_1 f_1(x)$ for all $x \in \mathbb{R}$.] As in Pukelsheim and Studden [(1993), page 410], it follows that

$$\begin{aligned} \lambda_{\min}\Big[C_{K_2}\big(M_2(\xi)\big)\Big] &\le z_2' L_2 M_2(\xi) L_2' z_2 \\ &= \int \omega(x) x^2 \big(z_1' L_1 f_1(x)\big)^2 \, d\xi(x) \\ &\le \int \omega(x) \big(z_1' L_1 f_1(x)\big)^2 d\xi(x) = z_1' L_1 M_1(\xi) L_1' z_1 \\ &= \lambda_{\min}\Big[C_{K_1}\big(M_1(\xi)\big)\Big]. \end{aligned} \tag{6}$$

Notice that the condition $b \le 1$ becomes important in the last inequality of (6).

Equality in (6) entails $\omega(x)(1 - x^2)(z_1' L_1 f_1(x))^2 = 0$ for all $x \in \operatorname{supp}(\xi)$. Thus, if $b < 1$ and $M(\xi)$, and hence $C_K(M(\xi))$, are regular, then ξ has (at least) $d + 1$ support points in $\{x : \omega(x) \neq 0\}$, all of which are zeros of the polynomial $z_1' L_1 f_1$. Now, $\operatorname{degree}(z_1' L_1 f_1) \le d - 1$ gives $z_1' L_1 f_1 \equiv 0$, hence $\lambda_{\min}[C_{K_1}(M_1(\xi))] = 0$, contrary to the regularity of $C_{K_1}(M_1(\xi))$. □

We will characterize E-optimality for $K\theta = (\vartheta_i)_{i \in \mathcal{J}}$ in the following two setups:

(A) $a \ge 0$, where $\mathcal{J} \neq \{0\}$ or $a > 0$.

(B) $\mathcal{J}$ fulfills (5), $a = -b$ with $b \le 1$ and $\omega(x) = \omega(-x), x \in [-b, b]$, where in the case $b = 1$ either $\omega \equiv 1$ or ω is one of the weight functions considered in Lemma 4.

We note that for the constant weight function $\omega \equiv 1$ conditions (A) and (B) are also considered in Pukelsheim and Studden (1993).

THEOREM 7. *Let either* (A) *or* (B) *be fulfilled, and suppose that there exists a solution p_0 to* (1) *with at most $d + 1$ global maxima in $[a, b]$. Then the E-optimal design ξ_0 for $K\theta$ is supported by the $d + 1$ extrema $b \ge x_0 > \cdots > x_d \ge a$ in $[a, b]$ of the polynomial $R = \sqrt{\omega} r' f$ which, in case* (A) *is the only equioscillating polynomial over $[a, b]$ with leading coefficient $r_d = 1$, and in case* (B) *is the only equioscillating polynomial over $[-b, b]$ with leading coefficient $r_d = 1$, and $R(x) = (-1)^d R(-x)$ for all $x \in [-b, b]$.*

In both cases, ξ_0 *is given by*

$$\xi_0(x_\nu) = (-1)^\nu \alpha\, e_\nu' W^{-1/2} F^{-1} K'Kr/\|Kr\|^2, \qquad 0 \le \nu \le d,$$

with $F = (x_\nu^\mu)_{0 \le \mu, \nu \le d}$, $W = \mathrm{diag}_{0 \le \nu \le d}(\omega(x_\nu))$ *and* $\alpha = \max_{x \in [a,b]}|R(x)|$, *and* Kr *is an eigenvector of* $C_K(M(\xi_0))$ *to the smallest eigenvalue* $\alpha^2\|Kr\|^{-2}$.

PROOF. (i) We start with setup (A). It follows from Theorem 1 and Lemma 5 that ξ_0 is supported by exactly $d+1$ points $b \ge x_0 > \cdots > x_d \ge a$, all of which are global maxima of p_0 in $[a,b]$. The information matrix $C_K(M_0), M_0 = M(\xi_0)$, is regular, and by Heiligers [(1994), Lemma 4] this matrix has a simple smallest eigenvalue $\lambda_0 > 0$. Let $z = (z_0, \dots, z_{s-1})'$ be a corresponding normalized eigenvector. Then $p_0 = (\sqrt{\omega} z' L_0 f)^2$ for some $L_0 \in \mathcal{G}_{K'}$, where the polynomial $\widetilde{R} = \sqrt{\omega} z' L_0 f$ has the property that

$$|\widetilde{R}(x)| \le |\widetilde{R}(x_\nu)| = \sqrt{\lambda_0} \quad \text{for all } x \in [a,b] \text{ and all } 0 \le \nu \le d. \tag{7}$$

The sequence $\widetilde{R}(x_\nu)$, $0 \le \nu \le d$, alternates in sign, as can be seen as follows. From equation (2) in the proof of Theorem 2 we get that $\widetilde{R}(x_\nu)$ and $e_\nu' W^{-1/2} \times F^{-1}K'z$ have the same sign. Let $i_0 < \cdots < i_{s-1}$ be the elements of $\mathcal{I}$, arranged according to increasing values. Lemma 4 in Heiligers (1994) implies that there are exactly $s-1$ sign changes in the sequence $(-1)^{i_\ell - \ell} z_\ell$, $0 \le \ell \le s-1$, where none of the coordinates z_ℓ vanishes; therefore we may assume that $\mathrm{sgn}(z_\ell) = (-1)^{d - i_\ell}$, $0 \le \ell \le s-1$. Moreover, Theorem 8.12.4 in Graybill (1983) yields for the entries $g_{\mu,\nu}$, $0 \le \mu, \nu \le d$, of the inverse of F that $\mathrm{sgn}(g_{\mu,\nu}) = (-1)^{d+\mu+\nu}$ and that at most the first column of F^{-1} may contain zeros. Hence, for all $0 \le \nu \le d$,

$$\begin{aligned} \mathrm{sgn}\big(\widetilde{R}(x_\nu)\big) &= \mathrm{sgn}\big(e_\nu' W^{-1/2} F^{-1} K'z\big) \\ &= \mathrm{sgn}\left(\sum_{\ell=0}^{s-1} \big(\omega(x_\nu)\big)^{-1/2} g_{\nu, i_\ell} z_\ell\right) = (-1)^\nu. \end{aligned} \tag{8}$$

In addition, from (7) and (8) we find, for the vector $\widetilde{r}$ of coefficients of $\widetilde{R}$,

$$\widetilde{r} = (F')^{-1} W^{-1/2} \big(\widetilde{R}(x_\nu)\big)_{0 \le \nu \le d} = \sqrt{\lambda_0} (F')^{-1} W^{-1/2} \big((-1)^\nu\big)_{0 \le \nu \le d};$$

in particular, reasoning as above, it follows that the leading coefficient $\widetilde{r}_d$ is different from zero with $\mathrm{sgn}(\widetilde{r}_d) = 1$. Hence, the polynomial $R = \widetilde{r}_d^{-1} \widetilde{R} = \sqrt{\omega} r' f$ has leading coefficient 1 and possesses the equioscillating property

$$|R(x)| \le \sqrt{\lambda_0}/\widetilde{r}_d = (-1)^\nu R(x_\nu) \quad \text{for all } x \in [a,b] \text{ and all } 0 \le \nu \le d.$$

Note that $\widetilde{r}_d \|Kr\| = \|K\widetilde{r}\| = \|z\| = 1$; thus $\sqrt{\lambda_0} = \max_{x \in [a,b]} |R(x)|/\|Kr\|$.

Inserting (7) and (8) into the formula for the weights of ξ_0 given in Theorem 2 and observing that $K'z = K'K\widetilde{r}$, we obtain

$$\begin{aligned} M_0 r &= F W^{1/2} \mathrm{diag}_{0 \le \nu \le d}\big(\lambda_0 e_\nu' W^{-1/2} F^{-1} K'z / \widetilde{R}(x_\nu)\big) W^{1/2} F' r \\ &= \widetilde{r}_d^{-1} \lambda_0 F W^{1/2} \mathrm{diag}_{0 \le \nu \le d}\big((-1)^\nu e_\nu' W^{-1/2} F^{-1} K'z\big) \big((-1)^\nu\big)_{0 \le \nu \le d} \\ &= \lambda_0 K'Kr, \end{aligned} \tag{9}$$

and the theorem in Krafft (1983) yields

$$C_K(M_0)Kr = \lambda_0 Kr.$$

Finally, let $\widehat{R} = \sqrt{\omega}\widehat{r}'f$ be a (further) equioscillating polynomial in $\sqrt{\omega}x^\mu, 0 \leq \mu \leq d$, with $\widehat{r}_d = 1$, and fix associated points $b \geq \widehat{x}_0 > \cdots > \widehat{x}_d \geq a$ such that the following hold:

$$(10)\qquad \begin{aligned} |\widehat{R}(x)| \leq |\widehat{R}(\widehat{x}_\nu)| \quad (=\widehat{\beta}, \text{ say}) \text{ for all } x \in [a, b] \text{ and all } 0 \leq \nu \leq d,\\ \widehat{R}(\widehat{x}_\nu)\widehat{R}(\widehat{x}_{\nu+1}) < 0 \quad \text{for all } 0 \leq \nu < d. \end{aligned}$$

Consider the c-optimal design $\widehat{\xi}$ within the set of designs supported by $\{\widehat{x}_0, \dots, \widehat{x}_d\}$, where $c = K'K\widehat{r}$,

$$\widehat{\xi}(\widehat{x}_\nu) = \widehat{\gamma}\widehat{\beta}^{-1}\left|e_\nu'\widehat{W}^{-1/2}\widehat{F}^{-1}K'K\widehat{r}\right|, \qquad 0 \leq \nu \leq d$$

[cf. Pukelsheim and Torsney (1991)]. Here $\widehat{\gamma}$ is a normalizing constant and the matrices $\widehat{F}$ and $\widehat{W}$ are defined as F and W, respectively, with x_ν replaced by $\widehat{x}_\nu$. Relation (10) implies that $\widehat{W}^{1/2}\widehat{F}'\widehat{r} = \pm\widehat{\beta}((-1)^\mu)_{0 \leq \mu \leq d}$, and therefore, arguing as above, the coordinates of $\widehat{r}$ must alternate in sign, where the $\widehat{r}_\mu, \mu \geq 1$, do not vanish. Consequently, $\widehat{r}_d = 1$ ensures $\operatorname{sgn}(\widehat{r}_\mu) = (-1)^{d-\mu}$ for all μ; hence $\operatorname{sgn}(e_\nu'\widehat{W}^{-1/2}\widehat{F}^{-1}K'K\widehat{r}) = (-1)^\nu$ for all $0 \leq \nu \leq d$. As in (9) it follows that

$$(11)\qquad \begin{aligned} M(\widehat{\xi})\widehat{r} = \widehat{\gamma}K'K\widehat{r} \quad \text{and}\\ K\widehat{r} \text{ is an eigenvector of } C_K\big(M(\widehat{\xi})\big) \text{ to the eigenvalue } \widehat{\gamma}. \end{aligned}$$

The sequence $\operatorname{sgn}((-1)^{i_\ell - \ell}\widehat{r}_{i_\ell}) = (-1)^\ell$, $0 \leq \ell \leq s-1$, alternates in sign, and by Heiligers [(1994), Lemma 4] $\widehat{\gamma}$ is the smallest eigenvalue of $C_K(M(\widehat{\xi}))$. Premultiplication of (11) by $\widehat{r}'$ yields

$$\widehat{\gamma} = \frac{\int \widehat{R}^2(x)\, d\widehat{\xi}(x)}{\|K\widehat{r}\|^2} = \frac{\widehat{\beta}^2}{\|K\widehat{r}\|^2}.$$

Now, E-optimality of $\widehat{\xi}$ for $K\theta$ follows from

$$\begin{aligned} \|K\widehat{r}\|^2\lambda_{\min}\left[C_K\big(M(\widehat{\xi})\big)\right] &= \max_{x \in [a,b]} \widehat{R}^2(x) \geq \widehat{r}'M(\xi)\widehat{r}\\ &\geq \widehat{r}'K'C_K\big(M(\xi)\big)K\widehat{r}\\ &\geq \|K\widehat{r}\|^2\lambda_{\min}\left[C_K\big(M(\xi)\big)\right] \quad \text{for all designs } \xi. \end{aligned}$$

Consequently, Theorem 2 gives $\widehat{\xi} = \xi_0$; thus $\widehat{x}_\nu = x_\nu$, for all ν, and $\widetilde{R} = R$.

(ii) Consider setup (B), first with $b < 1$ or $\mathcal{J}_1 = \emptyset$ (with $\mathcal{J}_1$ defined as above). Again, $\operatorname{supp}(\xi_0) = \mathcal{E}(p_0)$ has cardinality $d + 1$, and is symmetric around zero; $\lambda_{\min}\,[C_K(M(\xi_0))]$ is a simple eigenvalue and $Z_0 = zz'$, where the eigenvector z

to the smallest eigenvalue of $C_K(M(\xi_0))$ corresponds to $C_{K_2}(M_2(\xi_0))$ (as follows in the case $\mathcal{I}_1 \neq \emptyset$ from Lemma 6). Consequently, by Heiligers [(1994), Lemma 5] all coordinates of z associated with $C_{K_1}(M_1(\xi_0))$ vanish and the sequence $(-1)^{i_\ell - \ell} z_\ell$, $0 \le \ell \le s_2 - 1$, built from the remaining coordinates ($\mathcal{I}_2 = \{i_0, \dots, i_{s_2-1}\}$, $i_0 < \cdots < i_{s_2-1}$) alternates in sign. (In particular, p_0 must be an even polynomial). Now the assertions can be verified as in case (i), where the crucial equation (8) is implied by the sign pattern of the nonvanishing coordinates of z and of the corresponding entries of the inverse of F, which is derived in Pukelsheim and Studden [(1993), page 407].

(iii) It remains to investigate the case $b = 1$ (and $\mathcal{I}_1 \neq \emptyset$). Let $\{b_n\}_{n \in \mathbb{N}}$ be a sequence of nonnegative numbers $b_n < 1$ with $\lim_{n\to\infty} b_n = 1$. It follows from part (ii), above, that the E-optimal designs ξ_n on $[-b_n, b_n]$ for $K\theta$ are supported by the $d+1$ extrema of the only equioscillating polynomials $R_n = \sqrt{\omega} r_n' f$ over $[-b_n, b_n]$ with leading coefficient 1 and $R_n(x) = (-1)^d R_n(-x)$ for all x. We may assume that the sequence $\{\xi_n\}_{n\in\mathbb{N}}$ converges to a design on $[-1,1]$, ξ_0, say, which is symmetric, since the ξ_n have this property. ξ_0 is easily found to be E-optimal for $K\theta$. Because Lemma 5 ensures regularity of $M(\xi_0)$ we obtain from Theorem 1 that

$$\lim_{n\to\infty} \lambda_{\min}\Big[C_K\big(M(\xi_n)\big)\Big] = \lambda_0 = \lambda_{\min}\Big[C_K\big(M(\xi_0)\big)\Big]$$
$$= \lim_{n\to\infty} \max_{x\in[-b_n, b_n]} \omega(x)\left(\frac{r_n' f(x)}{\|Kr_n\|}\right)^2.$$

In particular, boundedness of the sequence $\{r_n/\|Kr_n\|\}_{n\in\mathbb{N}}$ follows, which we may therefore assume to converge to $\tilde{r}$, say. Obvious limiting arguments yield for the polynomial $\tilde{R}(x) = \sqrt{\omega(x)}\tilde{r}' f(x)$, $x \in [-1,1]$, that

$$\big|\tilde{R}(x)\big| \le \big|\tilde{R}(x_\nu)\big| = \sqrt{\lambda_0} \quad \text{for all } x \in [a,b] \text{ and all } 0 \le \nu \le d,$$
$$\tilde{R}(x_\nu)\tilde{R}(x_{\nu+1}) < 0 \qquad \text{for all } 0 \le \nu < d,$$

and the proof can be completed as above. □

The equioscillation property of the polynomial R from Theorem 7 means that this polynomial solves the *linear* Chebyshev approximation problem:

> minimize $\max_{x\in[a,b]} |Q(x)|$ over all polynomials $Q(x) = \Sigma_{\mu=0}^d q_\mu \sqrt{\omega(x)} x^\mu$ with leading coefficient $q_d = 1$ [and $Q(x) = (-1)^d Q(-x)$ for all x in case (B)].

[See, e.g., Jones and Karlovitz (1970), page 139.] In addition, Theorem 7 ensures that R is the *only oscillating* solution to the linear problem. Uniqueness of this polynomial is not obvious, since ω may have zeros in $[a,b]$, and therefore $\sqrt{\omega(x)} x^\mu$, $0 \le \mu \le d$, may form a weak, but not a strict Chebyshev system over $[a,b]$. [Actually, if ω is strictly positive, then R is the only equioscillating polynomial among *all* polynomials with leading coefficient 1, in case (A) as well as in case (B).] Due to the uniqueness, R might be computed (numerically), for example by using the algorithms of Remes [see, e.g., Watson (1980), Section 3.5]. In some cases explicit solutions can be given. For example, for setups (A) and (B) we have $R(x) = \gamma T_d(h(x))$ in the case $\omega \equiv 1$, and $R(x) = \delta\sqrt{\omega}U_d(h(x))$ in the case $\omega(x) = (x-a)(b-x)$, where T_d and U_d are the Chebyshev polynomials of degrees d of the first and second kind; h is the bijective affine linear mapping transforming the interval $[-1, 1]$ onto $[a, b]$; and γ and δ are suitable normalizations. Thus, as special cases we obtain from Theorem 7 some of the results on E-optimality given in Pukelsheim and Studden (1993) and Dette (1993). A simple continuity argument shows that, for *some* nonsymmetric regions $[a, b]$ having zero as an interior point and for *some* symmetric regions $[-b, b]$ with $b \geq 1$, the designs defined as in Theorem 7 are E-optimal for $K\theta$ [see Heiligers (1992), page 61]. However, an example showing that these designs are *not* E-optimal for *all* symmetric regions $[-b, b]$ in case $K\theta = \theta$ (and $\omega \equiv 1$) is given in Dette and Studden [(1993), Example 5]; see also Dette (1993). Lemma 8 gives an analogous statement for all functions $\omega = \omega_b$ of the form $\omega_b(x) = \omega_1(x/b)$, $x \in [-b, b]$, where ω_1 is some fixed symmetric weight function over $[-1, 1]$.

Let $R = \sqrt{\omega_1}r'f$ be an equioscillating polynomial over $[-1, 1]$ with $R(x) = (-1)^d R(-x)$ for all x and positive leading coefficient, normalized so that $\max_{x\in[-1,1]} R(x) = 1$. Fix associated extreme points $1 \geq x_0 > \cdots > x_d \geq -1$ with $x_\nu = -x_{d-\nu}$, and set $F = (x_\nu^\mu)_{0\leq\mu,\nu\leq d}$, $W = \operatorname{diag}_{0\leq\nu\leq d}(\omega_1(x_\nu))$ and $H_b = \operatorname{diag}_{0\leq\nu\leq d}(b^{-\nu})$. By Theorem 7 the candidate for an E-optimal design over $[-b, b]$ for $K\theta = \theta$ (and weight function ω_b) is ξ_b given by

$$\xi_b(bx_\nu) = \lambda_b(-1)^\nu e_\nu' W^{-1/2}F^{-1}H_b^2 r, \qquad 0 \leq \nu \leq d, \tag{12}$$

where $\lambda_b = \left(\sum_{\nu=0}^d (-1)^\nu e_\nu' W^{-1/2}F^{-1}H_b^2 r\right)^{-1}$. [Actually, as in the proof of Theorem 7, the nonvanishing coordinates of r are found to alternate in sign, and thereby the sign pattern of the entries of F^{-1} implies that the numbers on the r.h.s. of (12) are positive.] It is easily seen that ξ_b is symmetric and that $H_b r$ is an eigenvector of $M(\xi_b)$ to the eigenvalue λ_b. Due to the sign changes of the sequence of nonvanishing coordinates, $H_b r$ corresponds to $\lambda_{\min}[M_2(\xi_b)]$. Consequently, λ_b is either the smallest or the second smallest eigenvalue of $M(\xi_b)$; it is the smallest eigenvalue iff $M(\xi_b) - \lambda_b I_{d+1}$ is nonnegative definite, equivalently, iff, with $\Pi = \operatorname{diag}_{0\leq\nu\leq d}((-1)^\nu)$,

$$\begin{aligned} D_b &= \Pi W^{-1/2}F^{-1}H_b\big(M(\xi_b) - \lambda_b I_{d+1}\big)H_b(F^{-1})'W^{-1/2}\Pi \\ &= \operatorname{diag}_{0\leq\nu\leq d}\big(\xi_b(bx_\nu)\big) - \lambda_b \Pi W^{-1/2}F^{-1}H_b^2(F^{-1})'W^{-1/2}\Pi \end{aligned}$$

is nonnegative definite.

LEMMA 8. *Let $d \geq 2$. Then, for sufficiently large $b > 0$ the design ξ_b given by (12) is* not *E-optimal for θ on $[-b, b]$ and weight function ω_b.*

PROOF. As an example, we consider the case of an odd regression degree $d = 2m + 1$ only. Denote the elements of $\Pi W^{-1/2}F^{-1}H_b^2(F^{-1})'W^{-1/2}\Pi$

by $v_{\mu,\nu;b}, 0 \leq \mu, \nu \leq d$. Let $1_{d+1} \in \mathbb{R}^{d+1}$ consist of 1's at all positions. By the equioscillation and normalization of R we have $\Pi 1_{d+1} = W^{1/2}F'r$; thus $D_b 1_{d+1} = 0$ and

$$\begin{aligned} 0 &= 1'_{d+1} D_b 1_{d+1} \\ &= 1 - \lambda_b \left(\sum_{0 \leq \mu, \nu \leq m} v_{\mu,\nu;b} + \sum_{m+1 \leq \mu, \nu \leq d} v_{\mu,\nu;b} + 2 \sum_{\substack{0 \leq \mu \leq m \\ m+1 \leq \nu \leq d}} v_{\mu,\nu;b} \right). \end{aligned}$$

Denoting by $c' = (1'_{m+1}, -1'_{m+1})$ the vector consisting of 1's at the first $m + 1$, and -1's at the remaining positions, it follows that

$$\begin{aligned} &\lambda_b^{-1} b^{2d} c' D_b c \\ &= \lambda_b^{-1} b^{2d} \left(1 - \lambda_b \left(\sum_{0 \leq \mu, \nu \leq m} v_{\mu,\nu;b} + \sum_{m+1 \leq \mu, \nu \leq d} v_{\mu,\nu;b} - 2 \sum_{\substack{0 \leq \mu \leq m \\ m+1 \leq \nu \leq d}} v_{\mu,\nu;b} \right) \right) \\ &= 4 \sum_{\substack{0 \leq \mu \leq m \\ m+1 \leq \nu \leq d}} b^{2d} v_{\mu,\nu;b} \quad [=q(b), \text{ say}]. \end{aligned}$$

Using Theorem 8.12.4 in Graybill (1983) and observing that $x_\mu = -x_{d-\mu}$ for all μ, the numbers in the latter sum are found to be

$$b^{2d} v_{\mu,\nu;b} = \left(1 - b^2 x_\mu x_{d-\nu}\right) \frac{\sum_{\ell=0}^{m} a_{\mu,\ell} a_{d-\nu,\ell} b^{2d-4\ell-2}}{|P_\mu(x_\mu) P_{d-\nu}(x_{d-\nu})| \sqrt{\omega_1(x_\mu)\omega_1(x_{d-\nu})}},$$

with

$$P_\mu(x) = (x + x_\mu) \prod_{\substack{\ell=0 \\ \ell \neq \mu}}^{m} (x^2 - x_\ell^2) = (x + x_\mu) \sum_{\ell=0}^{m} (-1)^{m-\ell} a_{\mu,\ell} x^{2\ell}, \qquad 0 \leq \mu \leq m,$$

where all coefficients $a_{\mu,\ell}$ are positive. Hence, q (considered as a function of b) is a polynomial of degree$(q) = 2d$ and leading coefficient

$$-4 \sum_{\mu=0}^{m} \sum_{\nu=m+1}^{d} \frac{x_\mu x_{d-\nu} a_{\mu,0} a_{d-\nu,0}}{|P_\mu(x_\mu) P_{d-\nu}(x_{d-\nu})| \sqrt{\omega_1(x_\mu)\omega_1(x_{d-\nu})}} < 0.$$

Therefore, for sufficiently large $b > 0, D_b$ is not nonnegative definite. □

When assuming that the smallest eigenvalue of the moment matrix $M(\xi_0)$ of an E-optimal design ξ_0 on $[-b, b]$ for θ has multiplicity 1, then, by arguments as in part (ii) in the proof of Theorem 7, ξ_0 and ξ_b defined as in (12) must coincide. Thus, Lemma 8 implies that for sufficiently large $b > 1$ the smallest eigenvalue of $M(\xi_0)$ has multiplicity 2 and corresponds to both submatrices $M_1(\xi_0)$ and $M_2(\xi_0)$.

Acknowledgment. I am grateful for the referees' careful reading and for their very helpful remarks and comments on this paper.

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