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MAXIMIN DESIGNS FOR EXPONENTIAL GROWTH MODELS AND HETEROSCEDASTIC POLYNOMIAL MODELS

BY LORENS A. IMHOF

Stanford University

This paper is concerned with nonsequential optimal designs for a class of nonlinear growth models, which includes the asymptotic regression model. This design problem is intimately related to the problem of finding optimal designs for polynomial regression models with only partially known heteroscedastic structure. In each case, a straightforward application of the usual D-optimality criterion would lead to designs which depend on the unknown underlying parameters. To overcome this undesirable dependence a maximin approach is adopted. The theorem of Perron and Frobenius on primitive matrices plays a crucial role in the analysis.

1. Introduction.

Consider the exponential growth model

$$y(x) = \exp(-\theta x^p) \sum_{k=0}^{n} \beta_k x^k + \varepsilon, \qquad x \in \mathscr{X}, \tag{1.1}$$

where $y(x)$ is the response to the control variable x, $\mathscr{X} \subset \mathbb{R}$ is the design space, $\beta_0, \dots, \beta_n$ and θ are the model parameters that are to be estimated, $p \in \{1, 2\}$ and ε, the random error, is normally distributed with mean zero and variance $\sigma^2 > 0$. Applications of growth models of this type abound [cf. Seber and Wild (1989)] and much recent attention has been devoted to the construction of optimal designs for model (1.1) and special cases of that model [e.g., Pronzato and Walter (1988), Chaloner (1993), Dette and Sperlich (1994), Mukhopadhyay and Haines (1995), Dette and Neugebauer (1996, 1997) and Dette and Wong (1996, 1998)]. From the design point of view, the salient feature of model (1.1) is its nonlinearity. For nonlinear models, the information matrix depends on the unknown parameters so that most tools of experimental design, as described, for example, in Pukelsheim (1993), cannot be applied. A natural way to choose designs that accommodate the dependence on the parameters is to use Bayesian or maximin optimality criteria; see Silvey (1980) and Ford, Titterington and Kitsos (1989). Almost all of the papers cited above use a Bayesian approach. This paper is concerned with designs for the exponential model which are D-optimal in a maximin sense. Only nonsequential designs are considered.

The nonlinear design problems are attacked by first determining D-optimal designs for suitably chosen polynomial heteroscedastic models. Specifically,

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consider

$$y(x) = \sum_{k=0}^{n} \beta_k x^k + \varepsilon(x;\theta), \qquad x \in \mathscr{X}, \tag{1.2}$$

where $\beta_0, \ldots, \beta_n$ are to be estimated and the random error $\varepsilon(x;\theta)$ is normally distributed with mean zero and variance $\sigma^2/\lambda(x;\theta)$. Here $\lambda(x;\theta)$, the efficiency function, is assumed only to belong to a known class of functions $\{\lambda(x;\theta): \theta \in \Theta\}$, the value of θ is unknown. Again, the uncertainty in θ is dealt with by a maximin approach. Optimal designs for this model are of interest in their own right and the present results complement recent findings of Huang, Chang and Wong (1995) and in particular those of Chang and Lin (1997). As a by-product, a conjecture of Chang and Lin is shown to be true. The point to notice is that even a slightly inaccurate specification of the efficiency function can lead to poor designs, as was observed by Dette and Wong (1996). Consider, by way of illustration, model (1.2) with $n = 3$ and efficiency function $\lambda(x;\theta) = \exp(-\theta x)$, $x \in \mathscr{X} = [0, \infty)$. If the true value of θ is 0.3 and one uses the design that is D-optimal for $\theta = 0.5$, then the resulting efficiency (cf. Section 2) of the design used is about 0.72. Had one instead assumed that $\theta \in [0.2, 0.8]$ and used the maximin design given in Theorem 3.1, then the resulting efficiency would have been 0.84.

Several approaches to finding minimax or maximin designs have been suggested in the literature. They are, however, only of indirect use in the present situation. The general algorithm of Wong (1992) for generating minimax optimal designs is tailored to linear models with known error structure and cannot be applied here. The geometric approach of Haines (1995) is applicable but is restricted to one-parameter models. The geometric method developed by Imhof and Wong (2000) is helpful in finding candidate designs, but does not yield analytical solutions and is restricted to the case where Θ contains only two points.

This paper is organized as follows. The design setting and the optimality criteria are described in Section 2. Optimal designs for polynomial models with various heteroscedastic structures are presented in Section 3. These designs are given in terms of orthogonal polynomials. Section 4 addresses design problems that arise from those of Section 3 by imposing an additional restriction on the design space. In this case, the optimal designs are given in terms of polynomials whose coefficients are themselves polynomials which satisfy a three-term recurrence formula similar to that for orthogonal polynomials. Here the theorem of Perron and Frobenius on primitive matrices is the crucial tool to verify optimality of a candidate design. In Section 5 it is shown how the results of Sections 3 and 4 can be used to obtain optimal designs for the exponential growth models.

2. Preliminaries. An approximate design for model (1.2) is represented by a probability measure ξ on $\mathscr{X}$. Only approximate nonsequential designs will be considered. If ξ has finite support, $\{x_1, \ldots, x_k\}$ say, then the observations on $y(x)$ are made at the support points with frequencies proportional to $\xi(x_1), \dots, \xi(x_k)$. All observations are assumed to be uncorrelated. Associated with each observation on $y(x)$ is the Fisher information matrix,

$$I(x;\theta) = f_n(x) f_n^T(x) \lambda(x;\theta),$$

where $f_n(x) = (1, x, \dots, x^n)^T$. The information matrix of a design ξ is given by

$$M(\xi;\theta) = \int I(x;\theta)\, d\xi(x).$$

For any given value of θ, the locally D-optimal design ξ_θ is the design that maximizes $\det M(\xi;\theta)$ [cf. Chernoff (1953)]. Obviously, locally optimal designs depend on θ and so cannot be implemented unless θ is known exactly. In this paper it will only be assumed that θ belongs to a known parameter set Θ. A design will then be judged for each $\theta \in \Theta$ with respect to what is achievable for that θ. Specifically, for a given value of θ, the efficiency [Pukelsheim (1993), page 132] of a design ξ is

$$\left(\frac{\det M(\xi;\theta)}{\det M(\xi_\theta;\theta)} \right)^{1/(n+1)}.$$

A design ξ^* is said to be a standardized maximin D-optimal design [cf. Dette (1997)] if it maximizes the minimal efficiency, or, equivalently,

$$\inf_{\theta\in\Theta} \frac{\det M(\xi^*;\theta)}{\det M(\xi_\theta;\theta)} = \sup_{\xi} \inf_{\theta\in\Theta} \frac{\det M(\xi;\theta)}{\det M(\xi_\theta;\theta)}. \tag{2.1}$$

An optimal k-point design is a design that is optimal among all designs with k support points. Note that the optimality criterion defined by (2.1) is the maximin analog to the Bayesian Φ_1-criterion of Dette and Wong (1996).

The standardized maximin design is to be distinguished from the (nonstandardized) maximin D-optimal design, which maximizes $\inf_{\theta\in\Theta} \det M(\xi;\theta)$. This criterion reflects a cautious approach and judges a design by its behavior in the worst case. See Pronzato and Walter (1988) for a comparison of the two maximin concepts.

3. Maximin designs for heteroscedastic polynomial models. This section is concerned with optimal designs for model (1.2) with error structure modeled by efficiency functions of the following form:

1. $\lambda(x;\theta) = \exp(-\theta x), \qquad x \in [0,\infty),\ \theta > 0;$
2. $\lambda(x;\theta) = \exp(-\theta x^2), \qquad x \in \mathbb{R},\ \theta > 0;$
3. $\lambda(x;\alpha,\beta) = (1-x)^\alpha (1+x)^\beta, \qquad x \in [-1,1],\ \alpha,\beta > 0.$

The set of competing designs is restricted to designs with minimum support, that is, to designs with $n+1$ support points, where n is the degree of the regression polynomial. Recently established results for Bayesian criteria strongly suggest that one cannot expect closed form solutions to the design problem without that restriction; see, for example, Dette and Neugebauer (1997). Pukelsheim and Wilhelm (1995) pointed out that designs with as few support points as possible may well be of particular interest from a practical point of view. Moreover, the numerical examples in Section 5 suggest that an optimal $(n+1)$-point design is also optimal among all designs, provided that the domain in which the nonlinear parameter is known to lie is not too large.

THEOREM 3.1. *Consider model* (1.2) *with* $\mathscr{X} = [0, \infty)$ *and* $\lambda(x;\theta) = \exp(-\theta x)$. *Let* Θ *be a nonempty compact subset of* $(0,\infty)$ *and* $\theta_{\min} = \min\Theta$, $\theta_{\max} = \max\Theta$, $\theta_{\min} < \theta_{\max}$. *Let* $L_n^{(1)}(x)$ *denote the generalized Laguerre polynomial of degree n orthogonal with respect to the weight* xe^{-x} *on* $[0,\infty)$. *Then the standardized maximin D-optimal* $(n+1)$*-point design with respect to* Θ *puts equal masses at the zeros of*

$$xL_n^{(1)}\left(\frac{\theta_{\max}-\theta_{\min}}{\log\theta_{\max}-\log\theta_{\min}}x\right).$$

REMARK 3.1. The standardized maximin D-optimal $(n+1)$-point design for model (1.2) with $\mathscr{X} = \mathbb{R}$ and $\lambda(x;\theta) = \exp(-\theta x^2)$, $0 < \theta_{\min} \le \theta \le \theta_{\max}$ puts equal masses at the zeros of

$$H_{n+1}\left(x\sqrt{\frac{\theta_{\max}-\theta_{\min}}{\log\theta_{\max}-\log\theta_{\min}}}\right),$$

where $H_{n+1}(x)$ denotes the Hermite polynomial of degree $n+1$. This follows from Theorem 3.1 by a symmetry argument and the relation between Laguerre and Hermite polynomials.

REMARK 3.2. A simple calculation based on the monotonicity of the efficiency function shows that in the situation of Theorem 3.1, the nonstandardized maximin D-optimal design puts equal masses at the zeros of $xL_n^{(1)}(\theta_{\max}x)$.

THEOREM 3.2. *Consider model* (1.2) *with* $\mathscr{X} = [-1, 1]$ *and* $\lambda(x;\alpha,\beta) = (1-x)^{\alpha+1}(1+x)^{\beta+1}$. *Let* $\Theta \subset (-1,\infty)^2$ *be a compact convex body and let* Γ *denote the boundary of* Θ. *Let* $P_{n+1}^{(\alpha,\beta)}(x)$ *denote the Jacobi polynomial of degree* $n+1$ *orthogonal with respect to the weight* $(1-x)^\alpha(1+x)^\beta$ *on* $[-1,1]$. *Then the standardized maximin D-optimal* $(n+1)$*-point design with respect to* Θ *puts equal masses at the zeros of* $P_{n+1}^{(\alpha^*,\beta^*)}(x)$, *where* $(\alpha^*, \beta^*) \in (-1,\infty)^2$ *maximizes*

$$\min_{(u,v)\in\Gamma}\prod_{k=1}^{n+1}\left(\frac{k+\alpha}{k+u}\right)^{k+u}\left(\frac{k+\beta}{k+v}\right)^{k+v}\left(\frac{n+1+k+u+v}{n+1+k+\alpha+\beta}\right)^{n+1+k+u+v}.$$

In general, the optimal parameters α^* and β^* in Theorem 3.2 will have to be determined numerically. It is all the more remarkable that in the case where Θ is an interval of the form $[\alpha_{\min}, \alpha_{\max}]^2$, the solution to the maximin problem turns out to be particularly simple.

THEOREM 3.3. *Suppose that, in the situation of Theorem* 3.2, $\Theta = [\alpha_{\min}, \alpha_{\max}]^2$, $0 < \alpha_{\min} < \alpha_{\max}$. *Let* $P_{n+1}^{(\gamma)}(x)$ *denote the ultraspherical polynomial of degree* $n+1$ *orthogonal with respect to the weight* $(1-x^2)^{\gamma-\frac{1}{2}}$ *on* $[-1,1]$. *Then the standardized maximin* D-*optimal* $(n+1)$-*point design with respect to* Θ *puts equal masses at the zeros of*

$$P_{n+1}^{\left(\frac{1}{2}(\alpha_{\min}+\alpha_{\max}+1)\right)}(x).$$

To compare the maximin designs with optimal designs obtained by a Bayesian approach consider the setting of Theorem 3.1 with $\Theta = [1.0, 2.5]$ and the Bayesian criterion

$$\Phi(\xi) = \int_{\Theta} \left(\frac{\det M(\xi;\theta)}{\det M(\xi_\theta;\theta)} \right)^{1/(n+1)} d\pi(\theta).$$

Here ξ_θ is the locally D-optimal design and π, the prior distribution, is taken to be uniform on Θ. The Φ-optimal $(n+1)$-point designs are given in Dette and Wong (1996). Table 1 shows for $n = 2, 3, 4$ the design points, the minimum efficiency and the average efficiency of the maximin and the Φ-optimal $(n+1)$-point design. The performance of the Bayesian designs with respect to the minimax criterion agrees with the general observations of Pronzato and Walter (1988). The minimax designs are in these cases nearly Φ-optimal.

In the situation of Theorem 3.3, the maximin designs coincide with the Bayesian D-optimal design with respect to the uniform prior on Θ. If Θ contains only one point; that is, if the heteroscedastic structure of the underlying model is completely known, then the maximin designs coincide with the well-known D-optimal designs for weighted polynomial regression [see e.g. Proposition VI.6 in Pázman (1986)].

The proofs of Theorems 3.1 through 3.3 are similar and therefore only Theorem 3.3 will be proved here. That proof requires two auxiliary results, which are established in the Appendix.

TABLE 1

Support points, minimum and average efficiencies of minimax designs ξ_M *and Bayesian* Φ-*optimal designs* ξ_B *for model* (1.2) *with* $\mathscr{X} = [0, \infty)$, $\lambda(x;\theta) = \exp(-\theta x)$, $\theta \in \Theta = [1.0, 2.5]$

n			ξ_M			min-eff(ξ_M)	$\Phi(\xi_M)$
2	0.0	0.775	2.891			0.813	0.935
3	0.0	0.572	2.019	4.740		0.732	0.905
4	0.0	0.454	1.571	3.501	6.691	0.660	0.877
n			ξ_B			min-eff(ξ_B)	$\Phi(\xi_B)$
2	0.0	0.725	2.704			0.769	0.939
3	0.0	0.535	1.889	4.434		0.675	0.911
4	0.0	0.425	1.470	3.275	6.259	0.591	0.885

LEMMA 3.1. *Let* $y_1^{(\alpha,\beta)} < y_2^{(\alpha,\beta)} < \cdots < y_n^{(\alpha,\beta)}$ *denote the zeros of the Jacobi polynomial* $P_n^{(\alpha,\beta)}(y)$. *Then*

$$\left\{\left(\prod_{k=1}^{n}\left(1-y_k^{(\alpha,\beta)}\right), \prod_{k=1}^{n}\left(1+y_k^{(\alpha,\beta)}\right)\right): \alpha, \beta > -1\right\}$$
$$= \left\{\left(\prod_{k=1}^{n}(1-x_k), \prod_{k=1}^{n}(1+x_k)\right): \ -1 < x_1 < \cdots < x_n < 1\right\}.$$

LEMMA 3.2. *Let* $n \in \mathbb{N}$ *and* $s, t \geq 0$. *Then*

$$\prod_{k=1}^{n}\left(\frac{k+(s+t)/2}{k+s}\right)^{k+s}\left(\frac{k+t}{k+(s+t)/2}\right)^{k+t}\left(\frac{n+k+2s}{n+k+s+t}\right)^{n+k+2s} \geq 1$$

with equality if and only if $s = t$.

PROOF OF THEOREM 3.3. Note first that when $\xi_*^{(\alpha,\beta)}$ denotes the locally D-optimal design for (α, β), then

$$\det M(\xi_*^{(\alpha,\beta)}; \alpha, \beta)$$
$$= 2^{(n+1)(n+2+\alpha+\beta)} \prod_{k=1}^{n} k^k \prod_{k=1}^{n+1} \frac{(k+\alpha)^{k+\alpha}(k+\beta)^{k+\beta}}{(n+1+k+\alpha+\beta)^{n+1+k+\alpha+\beta}};$$

see Dette and Wong (1996), Lemma 3.1. Now let ξ be an arbitrary $(n+1)$-point design with support points $x_0, x_1, \ldots, x_n$ and weights $w_0, w_1, \ldots, w_n$. Then, by Lemma 5.1.3 in Silvey (1980),

$$\det M(\xi; \alpha, \beta) \leq \frac{1}{(n+1)^{n+1}} \prod_{k=0}^{n}(1-x_k)^{\alpha+1}(1+x_k)^{\beta+1} \prod_{0\leq\mu<\nu\leq n}(x_\mu - x_\nu)^2$$

with equality if and only if $w_k = 1/(n+1)$ for $k = 0, \ldots, n$. One may, of course, assume that $x_0 > -1$ and $x_n < 1$. In view of Lemma 3.1, there exist constants $\alpha' = \alpha'(\xi) > -1$ and $\beta' = \beta'(\xi) > -1$ such that the zeros $y_0, y_1, \ldots, y_n$ of $P_{n+1}^{(\alpha',\beta')}(y)$ satisfy

$$\prod_{k=0}^{n}(1-x_k) = \prod_{k=0}^{n}(1-y_k), \qquad \prod_{k=0}^{n}(1+x_k) = \prod_{k=0}^{n}(1+y_k).$$

It therefore follows by Szegö (1975), Theorems 6.7.1 and 6.71 and equations (4.1.1), (4.1.4) and (4.21.6) that

$$\prod_{k=0}^{n}(1-x_k)^{\alpha+1}(1+x_k)^{\beta+1}\prod_{\mu<\nu}(x_\mu - x_\nu)^2$$
$$\leq \prod_{k=0}^{n}(1-x_k)^{\alpha-\alpha'}(1+x_k)^{\beta-\beta'}$$

$$\times \prod_{k=0}^{n}(1-y_k)^{\alpha'+1}(1+y_k)^{\beta'+1}\prod_{\mu<\nu}(y_\mu-y_\nu)^2$$

$$= 2^{(n+1)(n+2+\alpha+\beta)}\prod_{k=1}^{n+1}\frac{k^k(k+\alpha')^{k+\alpha}(k+\beta')^{k+\beta}}{(n+1+k+\alpha'+\beta')^{n+1+k+\alpha+\beta}}.$$

Consequently,

$$\min_{(\alpha,\beta)\in\Theta}\frac{\det M(\xi;\alpha,\beta)}{\det M(\xi_*^{(\alpha,\beta)};\alpha,\beta)} \le \min_{(\alpha,\beta)\in\Theta} H(\alpha,\beta,\alpha',\beta'), \tag{3.1}$$

where

$$H(\alpha,\beta,u,v) = \prod_{k=1}^{n+1}\left(\frac{k+u}{k+\alpha}\right)^{k+\alpha}\left(\frac{k+v}{k+\beta}\right)^{k+\beta} \times \left(\frac{n+1+k+\alpha+\beta}{n+1+k+u+v}\right)^{n+1+k+\alpha+\beta}.$$

Moreover, there is equality in (3.1) if and only if ξ puts equal masses at the zeros of $P_{n+1}^{(\alpha',\beta')}(x)$.

Let $\alpha^* = \frac{1}{2}(\alpha_{\min}+\alpha_{\max})$. A brief calculation shows that

$$\begin{aligned}&\min\{H(\alpha_{\min},\alpha_{\max},\alpha',\beta'), H(\alpha_{\max},\alpha_{\min},\alpha',\beta')\}\\ &\quad < H\Big(\alpha_{\min},\alpha_{\max},\tfrac{1}{2}(\alpha'+\beta'),\tfrac{1}{2}(\alpha'+\beta')\Big)\end{aligned} \tag{3.2}$$

unless $\alpha'=\beta'$, and

$$H\Big(\alpha_{\min},\alpha_{\max},\tfrac{1}{2}(\alpha'+\beta'),\tfrac{1}{2}(\alpha'+\beta')\Big) < H\big(\alpha_{\min},\alpha_{\max},\alpha^*,\alpha^*\big) \tag{3.3}$$

unless $\frac{1}{2}(\alpha'+\beta')=\alpha^*$. It is straightforward to verify that $\log H(\alpha,\beta,\alpha^*,\alpha^*)$ is a strictly concave function of (α,β). The minimum subject to $(\alpha,\beta)\in\Theta$ is therefore attained at some extreme point of Θ, that is at $(\alpha_{\min},\alpha_{\min})$, $(\alpha_{\min},\alpha_{\max})$, $(\alpha_{\max},\alpha_{\min})$ or $(\alpha_{\max},\alpha_{\max})$. Obviously, $H(\alpha_{\min},\alpha_{\max},\alpha^*,\alpha^*) = H(\alpha_{\max},\alpha_{\min},\alpha^*,\alpha^*)$, and it follows from Lemma 3.2 that

$$\frac{H(\alpha_{\min},\alpha_{\min},\alpha^*,\alpha^*)}{H(\alpha_{\max},\alpha_{\min},\alpha^*,\alpha^*)} > 1, \qquad \frac{H(\alpha_{\max},\alpha_{\max},\alpha^*,\alpha^*)}{H(\alpha_{\max},\alpha_{\min},\alpha^*,\alpha^*)} > 1.$$

Hence,

$$\min_{(\alpha,\beta)\in\Theta} H(\alpha,\beta,\alpha^*,\alpha^*) = H(\alpha_{\min},\alpha_{\max},\alpha^*,\alpha^*). \tag{3.4}$$

Combining (3.1) through (3.4), one obtains that

$$\min_{(\alpha,\beta)\in\Theta}\frac{\det M(\xi;\alpha,\beta)}{\det M(\xi_*^{(\alpha,\beta)};\alpha,\beta)} \le H(\alpha_{\min},\alpha_{\max},\alpha^*,\alpha^*)$$

with equality if and only if ξ puts equal masses at the zeros of

$$P_{n+1}^{(\alpha^*,\alpha^*)}(x) = \frac{\Gamma(2\alpha^*+1)}{\Gamma(\alpha^*+1)}\frac{\Gamma(n+\alpha^*+2)}{\Gamma(n+2\alpha^*+2)}P_{n+1}^{\left(\alpha^*+\frac{1}{2}\right)}(x). \qquad \square$$

4. Maximin designs for heteroscedastic polynomial models on restricted design spaces. This section takes up the design problem of Theorem 3.1. Instead of the unbounded design space $\mathscr{X} = [0,\infty)$, the design space will now be a compact interval.

Again, let $L_n^{(1)}(x)$ denote the generalized Laguerre polynomial of degree n.

THEOREM 4.1. *Consider model* (1.2) *with* $\mathscr{X} = [0, b]$ *and* $\lambda(x;\theta) = \exp(-\theta x)$. *Let* Θ *be a nonempty compact subset of* $(0,\infty)$ *and* $\theta^* = \max\Theta$. *Define polynomials* $C_k(u)$ *recursively by* $C_{-1}(u) = 0$, $C_0(u) = 1$ *and*

$$\begin{aligned} b(k+1)(k+2)C_{k+1}(u) = {} & (k(k+3+b\theta^*)-u)C_k(u) \\ & + (n-k)\theta^* C_{k-1}(u) \end{aligned} \tag{4.1}$$

for $k = 0,\dots,n-1$. *Let* u^* *and* x^* *denote the largest zeros of* $C_n(u)$ *and* $L_n^{(1)}(x)$, *respectively*.

(a) *If* $x^* \le b\theta^*$, *then the maximin D-optimal design with respect to* Θ *puts equal masses at the zeros of* $xL_n^{(1)}(\theta^* x)$. *A sufficient condition for* $x^* \le b\theta^*$ *to hold is that* $n \le b\theta^*/4 + 1/2$.

(b) *If* $x^* > b\theta^*$, *then the maximin D-optimal design with respect to* Θ *puts equal masses at the* $n+1$ *zeros of*

$$x(b-x)\sum_{k=0}^{n-1} C_k(u^*)x^k.$$

A sufficient condition for $x^* > b\theta^*$ *to hold is that* $n \ge 4b\theta^*/\pi^2 + 3/4$.

REMARK 4.1. The corresponding design problem for model (1.2) with $\mathscr{X} = [-b, b]$ and $\lambda(x;\theta) = \exp(-\theta x^2)$ can be dealt with along similar lines. The details are omitted.

REMARK 4.2. Chang and Lin (1997) conjectured that for polynomial regression on $[-1, 1]$ with known efficiency function $\lambda(x) = \exp(\alpha x)$, there is a critical value $\alpha^* = \alpha^*(n)$ such that if S denotes the support of the D-optimal design, then $-1 \notin S$ and $+1 \in S$ if $\alpha > \alpha^*$; $\{-1,+1\} \subset S$ if $|\alpha| \le \alpha^*$; and $-1 \in S$ and $+1 \notin S$ if $\alpha < -\alpha^*$. That this is indeed the case follows from Theorem 4.1. Choose $\Theta = \{\theta\} = \{-\alpha\}$. Note that the theorem is easily extended to arbitrary intervals $\mathscr{X} = [a, b]$ and to negative θ. If $\xi(x)$ is D-optimal for $\lambda(x) = \exp(-\theta x)$, $x \in [0, b-a]$, then $\xi(x-a)$ is D-optimal for $\lambda(x) = \exp(-\theta x)$, $x \in [a, b]$ and $\xi(-x-a)$ is D-optimal for $\lambda(x) = \exp(+\theta x)$, $x \in [-b, -a]$. It now follows that the conjecture is correct and the critical value is the largest zero of $L_n^{(1)}(2\alpha)$. This ties in with the numerical values in Table 2 of Chang and Lin (1997).

Similarly, the critical value α^* in Table 4 of Chang and Lin (1997) is the smallest zero of $H_{n+1}(|-\alpha|^{1/2})$.

REMARK 4.3. Equation (4.1) is reminiscent of the three-term recurrence formula for orthogonal polynomials; see for example, Theorem 3.2.1 in Szegö (1975). However, the polynomials $C_0(u), \dots, C_n(u)$ do not form an orthogonal system, for if they did, the coefficients of $C_{k+1}(u)$ and $C_{k-1}(u)$ in (4.1) would have different signs. Moreover, in general the polynomials $F_{n-1}(x) = \sum_{k=0}^{n-1} C_k(u^*)x^k$, $n = 1, 2, \dots$, do not form an orthogonal system either. This can also be verified with Theorem 3.2.1 in Szegö (1975).

PROOF OF THEOREM 4.1. The first assertion of (a) is an immediate consequence of Theorem 3.1. If $n \le b\theta^*/4 + 1/2$, then, by inequality (13) in Sansone (1959), page 316, $x^* < 4n - 2 \le b\theta^*$, which completes the proof of (a). The second assertion of (b) follows from inequality (20_1) in Sansone [(1959), page 317] and a bound for the zeros of Bessel's function $J_1(x)$ [see Watson (1952), page 492].

Now suppose that $x^* > b\theta^*$. In order to determine the D-optimal design ξ^* for the efficiency function $\lambda(x; \theta^*) = \exp(-\theta^* x)$ note first that this design must have exactly $n+1$ support points, say $x_0 < x_1 < \cdots < x_n$, and that it must put equal masses at these points. This follows from Theorem 3.6 in Karlin and Studden [(1966), page 333] since $\{\exp(\theta^* x), 1, x, \cdots, x^{2n}\}$ is a Chebyshev system on $[0, b]$. Hence

$$\det M(\xi^*; \theta^*) = \frac{\exp(-\theta^*(x_0 + \cdots + x_n))}{(n+1)^{n+1}} \prod_{0 \le \mu < \nu \le n} (x_\mu - x_\nu)^2. \tag{4.2}$$

Obviously, $x_0 = 0$. If $x_n < b$, then an argument similar to that of Szegö [(1975), page 141] would yield that $x_1, \dots, x_n$ are the zeros of $L_n^{(1)}(\theta^* x)$. This would imply that $x_n = x^*/\theta^* > b$, which is impossible. Thus $x_n = b$. It then follows from (4.2) on differentiating with respect to $x_1, \dots, x_{n-1}$ that the polynomial $F(x) = (x - x_1) \cdots (x - x_{n-1})$ satisfies the differential equation

$$x(b-x)F''(x) + (2b - 4x - \theta^* x(b-x)) + (\rho - (n-1)\theta^* x)F(x) = 0 \tag{4.3}$$

for some $\rho \in \mathbb{R}$. Write $F(x) = \sum_{k=0}^{n-1} q_k x^k$ and $\mathbf{q} = (q_0, q_1, \dots, q_{n-1})^T$. Then (4.3) is equivalent to

$$A\mathbf{q} = \rho \mathbf{q}, \tag{4.4}$$

where

$$A = \begin{bmatrix} s_0 & t_0 & 0 & 0 & \dots & 0 & 0 & 0 \\ r_1 & s_1 & t_1 & 0 & \dots & 0 & 0 & 0 \\ 0 & r_2 & s_2 & t_2 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & r_{n-2} & s_{n-2} & t_{n-2} \\ 0 & 0 & 0 & 0 & \dots & 0 & r_{n-1} & s_{n-1} \end{bmatrix}$$

and

$$\begin{aligned} r_k &= (n-k)\theta^* > 0, \\ s_k &= k(k+3+\theta^* b) \geq 0, \\ t_k &= -b(k+1)(k+2) < 0. \end{aligned}$$

To determine the coefficient vector $\mathbf{q}$ set

$$B = \left(\binom{j}{i} b^{j-i} \right)_{i,j=0}^{n-1}.$$

Making use of the Vandermonde convolution formula [see Riordan (1968), page 8] one may verify that

$$P := BAB^{-1} = \begin{bmatrix} \tilde{s}_0 & -t_0 & 0 & 0 & \dots & 0 & 0 \\ r_1 & \tilde{s}_1 & -t_1 & 0 & \dots & 0 & 0 \\ 0 & r_2 & \tilde{s}_2 & -t_2 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & r_{n-1} & \tilde{s}_{n-1} \end{bmatrix}$$

where $\tilde{s}_k = k(k+3) + (n-1-k)\theta^* b > 0$. Thus P is a nonnegative matrix and it is easily seen that all the elements of P^{n-1} are positive. This means that P is a primitive matrix. It therefore follows from the theorem of Perron and Frobenius [Seneta (1981), page 3] that the largest characteristic root of P, the Perron–Frobenius root, is simple and that there is a corresponding positive characteristic vector, say $\mathbf{p}$. Note that all the characteristic roots of the Jacobi matrix P are real as $-t_k r_{k+1} > 0$ for all k. Moreover, every positive characteristic vector of P is proportional to $\mathbf{p}$. The vector $B\mathbf{q}$ is, by (4.4), a characteristic vector of P. The components of $B\mathbf{q}$ are the coefficients in the Taylor expansion of $F(x)$ around $x = b$. Consequently, as all the zeros of $F(x)$ are less than b, $B\mathbf{q}$ must be positive. Hence $B\mathbf{q}$ is proportional to $\mathbf{p}$.

On the other hand, it is easily seen by induction that

$$C_n(u) = \frac{\det(uI_n - A)}{t_0 t_1 \cdots t_{n-1}},$$

where I_n denotes the unit matrix of order n. Thus u^*, the largest zero of $C_n(u)$, is equal to the Perron–Frobenius root of P. Let $\mathbf{c} = (C_0(u^*), \dots, C_{n-1}(u^*))^T$. Then $A\mathbf{c} = u^*\mathbf{c}$, and so $PB\mathbf{c} = u^*B\mathbf{c}$. Since u^* is a simple characteristic root of P, $B\mathbf{c}$ must be proportional to $\mathbf{p}$, too. Therefore, $\mathbf{q}$ and $\mathbf{c}$ are proportional, and it follows that the design points $x_1, \dots, x_{n-1}$ are the zeros of $F(x) = q_0 \sum_{k=0}^{n-1} C_k(u^*)x^k$.

To complete the proof note that according to the basic composition formula [Karlin and Studden (1966), page 14] for any design ξ,

$$\det M(\xi;\theta) = \underset{y_0<\cdots<y_n}{\int \cdots \int} e^{-\theta\sum y_k}(\det[f_n(y_0), \dots, f_n(y_n)])^2 \, d\xi(y_0)\cdots d\xi(y_n),$$

showing that $\inf_{\theta\in\Theta} \det M(\xi;\theta) = \det M(\xi;\theta^*)$. Hence $\inf_\theta \det M(\xi^*;\theta) \geq \inf_\theta \det M(\xi;\theta)$ with equality if and only if $\xi = \xi^*$. □

REMARK 4.4. The matrix A in the proof of Theorem 4.1 is a Jacobi matrix with negative super- and positive subdiagonal entries so that the theorem of Perron and Frobenius cannot be applied directly. See Arscott (1961) for some results on matrices of that type.

5. Maximin designs for exponential growth models. Consider the growth model

$$y(x) = \exp(-\theta x)\sum_{k=0}^{n} \beta_k x^k + \varepsilon, \qquad x \in \mathscr{X} \tag{5.1}$$

where ε is normally distributed with constant variance and $\theta \in \Theta = [\theta_{\min}, \theta_{\max}]$, $0 < \theta_{\min} < \theta_{\max}$. Suppose interest is in estimating $\beta_0, \dots, \beta_n$ as well as θ. For this model, it was shown by Dette and Wong (1996) that the determinant of the Fisher information matrix of a design ξ is proportional to

$$\det N(\xi;\theta) = \det \int f_{n+1}(x) f_{n+1}^T(x) \exp(-2\theta x)\, d\xi(x).$$

The locally D-optimal design for $\theta, \beta_0, \dots, \beta_n$ depends therefore only on θ but not on $\beta_0, \dots, \beta_n$. The optimal designs for model (5.1) can now be obtained as an application of Theorems 3.1 and 4.1.

THEOREM 5.1. *Let x^* denote the largest zero of the generalized Laguerre polynomial $L_{n+1}^{(1)}(x)$.*

(a) *If $\mathscr{X} = [0,\infty)$ or $\mathscr{X} = [0,b]$ with $b \geq x^*/(2\theta_{\max})$, then the standardized maximin D-optimal $(n+2)$-point design for the growth model* (5.1) *puts equal masses at the zeros of*

$$xL_{n+1}^{(1)}\left(2\frac{\theta_{\max} - \theta_{\min}}{\log\theta_{\max} - \log\theta_{\min}}x\right) \tag{5.2}$$

and the nonstandardized maximin D-optimal design puts equal masses at the zeros of $xL_{n+1}^{(1)}(2\theta_{\max}x)$.

(b) *If* $\mathscr{X} = [0, b]$ *with* $b < x^*/(2\theta_{\max})$, *let* $C_{-1}(u) = 0$, $C_0(u) = 1$ *and, for* $k = 0, \dots, n$,

$$b(k+1)(k+2)C_{k+1}(u) = (k(k+3+2b\theta_{\max}) - u)C_k(u) + 2(n+1-k)\theta_{\max} C_{k-1}(u).$$

Denote the largest zero of $C_{n+1}(u)$ *by* u^*. *Then the maximin* D*-optimal design puts equal masses at the zeros of*

$$x(b-x)\sum_{k=0}^{n} C_k(u^*)x^k.$$

PROOF. It remains to consider the case where $\mathscr{X} = [0, b]$ and $b \geq x^*/(2\theta_{\max})$. Let Δ_1 and Δ_2 denote the set of all designs on $[0, b]$ and $[0, \infty)$, respectively. Then, for every $\theta \in \Theta$, the support of the locally D-optimal design in Δ_2 is, by Theorem 4.1, contained in $[0, b]$. Let ξ^* denote the design that puts equal masses at the zeros of the polynomial (5.2). An application of the mean value theorem to the function $\log \theta$ shows that

$$\frac{\theta_{\max} - \theta_{\min}}{\log \theta_{\max} - \log \theta_{\min}} \leq \theta_{\max},$$

which shows that $\xi^* \in \Delta_1$. Hence, again by Theorem 4.1,

$$\min_{\theta} \frac{\det N(\xi^*; \theta)}{\max_{\eta \in \Delta_1} \det N(\eta; \theta)} = \max_{\xi \in \Delta_2} \min_{\theta} \frac{\det N(\xi; \theta)}{\max_{\eta \in \Delta_2} \det N(\eta; \theta)} = \max_{\xi \in \Delta_1} \min_{\theta} \frac{\det N(\xi; \theta)}{\max_{\eta \in \Delta_1} \det N(\eta; \theta)}. \qquad \square$$

To assess the potential efficiency loss caused by restricting the number of support points, consider model (5.1) with $n = 0$, $\mathscr{X} = [0, \infty)$ and $0 < \theta_{\min} \leq \theta \leq \theta_{\max}$. Suppose that β_0 is known. It is then easily checked that the standardized maximin D-optimal one-point design puts all its mass at $\log(\theta_{\max}/\theta_{\min})/(\theta_{\max} - \theta_{\min})$. But to the model at hand one may also apply the geometric approach of Haines (1995). This yields that the one-point design is in fact optimal among all designs, not only among the one-point designs, provided that $\theta_{\max}/\theta_{\min} \leq (2 + \sqrt{3}) \approx 3.73$. It turns out that when the prior knowledge of θ is somewhat less accurate, that is, when $3.73 < \theta_{\max}/\theta_{\min} < 5$, say, then the efficiency loss caused by using the optimal one-point design instead of the optimal design is still small, although the two designs look quite different. If $\theta_{\max}/\theta_{\min}$ gets even larger, the efficiency loss does become noticeable, but the minimum efficiency of the optimal designs becomes low, too. Table 2 shows, for selected parameter intervals $[\theta_{\min}, \theta_{\max}]$, the optimal one-point design, the optimal design and their minimum efficiencies, where $\text{min-eff}(\xi) = \min_\theta e^2\theta^2 \int x^2 e^{-2\theta x}\, d\xi(x)$.

In light of this, it seems likely that there exist constants $c_n > 1$ such that the optimal $(n+2)$-point designs in Theorem 5.1 are optimal among all designs

TABLE 2

Optimal one-point designs ξ and optimal designs ξ^* for model (5.1) *with* $n = 0$, $\mathscr{X} = [0, \infty)$ *and* β_0 *known**

$[\boldsymbol{\theta}_{\min}, \boldsymbol{\theta}_{\max}]$	ξ	ξ^*		min-eff (ξ)	min-eff (ξ^*)
[1.0, 3.73]	0.482(1)	0.482(1)		0.655	0.655
[1.0, 4.0]	0.462(1)	0.427(0.866)	0.839(0.134)	0.626	0.627
[1.0, 5.0]	0.402(1)	0.263(0.615)	0.968(0.385)	0.535	0.570
[1.0, 6.0]	0.358(1)	0.199(0.565)	0.993(0.435)	0.463	0.547

*The support points are given with corresponding weights in parentheses.

as long as $\theta_{\max} \le c_n \theta_{\min}$. The problem of deriving explicit expressions for c_n or useful bounds remains open.

APPENDIX

PROOF OF LEMMA 3.1. Suppose that $n \ge 2$. Let

$$S_1 = \left\{ \left(\prod_{k=1}^{n} \left(1 - y_k^{(\alpha, \beta)}\right), \prod_{k=1}^{n} \left(1 + y_k^{(\alpha, \beta)}\right) \right) : \alpha, \beta > -1 \right\},$$

$$S_2 = \left\{ \left(\prod_{k=1}^{n} (1 - x_k), \prod_{k=1}^{n} (1 + x_k) \right) : \ -1 < x_1 < \cdots < x_n < 1 \right\},$$

$$S_3 = \left\{ (u, v) : u, v > 0, \ u^{1/n} + v^{1/n} < 2 \right\}.$$

Obviously, $S_1 \subset S_2$. If $(u, v) \in S_2$, then $u, v > 0$ and in view of the inequality of the arithmetic and geometric means,

$$\begin{aligned} u^{1/n} + v^{1/n} &= \prod_{k=1}^{n} (1 - x_k)^{1/n} + \prod_{k=1}^{n} (1 + x_k)^{1/n} \\ &< \frac{1}{n} \sum_{k=1}^{n} (1 - x_k) + \frac{1}{n} \sum_{k=1}^{n} (1 + x_k) \\ &= 2. \end{aligned}$$

Thus $S_2 \subset S_3$. To see that $S_3 \subset S_1$ note first that [cf. Szegö (1975), equations (4.1.1), (4.1.4), (4.21.6)]

$$\prod_{k=1}^{n} \left(1 - y_k^{(\alpha, \beta)}\right) = \frac{P_n^{(\alpha, \beta)}(1)}{l_n^{(\alpha, \beta)}} = 2^n \prod_{k=1}^{n} \frac{k + \alpha}{n + k + \alpha + \beta},$$

$$\prod_{k=1}^{n} \left(1 + y_k^{(\alpha, \beta)}\right) = 2^n \prod_{k=1}^{n} \frac{k + \beta}{n + k + \alpha + \beta},$$

where $l_n^{(\alpha,\beta)}$ denotes the leading coefficient of $P_n^{(\alpha,\beta)}(x)$. Now fix $(u, v) \in S_3$. Then for every $\alpha > -1$ there is a unique $\beta(\alpha) > -1$ such that

$$\frac{\prod_{k=1}^n \left(1 - y_k^{(\alpha,\beta(\alpha))}\right)}{\prod_{k=1}^n \left(1 + y_k^{(\alpha,\beta(\alpha))}\right)} = \frac{u}{v}.$$

As $\beta(\alpha)$ depends continuously on α, so does $y_k^{(\alpha,\beta(\alpha))}$; see Szegö (1975), page 115. Moreover,

$$\lim_{\alpha\to-1} \beta(\alpha) = -1, \qquad \lim_{\alpha\to\infty} \beta(\alpha) = \infty,$$
$$\lim_{\alpha\to\infty} \frac{\beta(\alpha)}{\alpha} = \lim_{\alpha\to\infty} \frac{\prod_{k=1}^n (1 + k/\alpha)^{1/n}}{\prod_{k=1}^n (1 + k/\beta(\alpha))^{1/n}} \left(\frac{v}{u}\right)^{1/n} = \left(\frac{v}{u}\right)^{1/n}.$$

Hence,

$$\lim_{\alpha\to-1} \prod_{k=1}^n \left(1 - y_k^{(\alpha,\beta(\alpha))}\right) = 0, \qquad \lim_{\alpha\to-1} \prod_{k=1}^n \left(1 + y_k^{(\alpha,\beta(\alpha))}\right) = 0$$

and

$$\lim_{\alpha\to\infty} \left(\prod_{k=1}^n \left(1 - y_k^{(\alpha,\beta(\alpha))}\right)^{1/n} + \prod_{k=1}^n \left(1 + y_k^{(\alpha,\beta(\alpha))}\right)^{1/n} \right)$$
$$= 2 \lim_{\alpha\to\infty} \frac{(1 + (v/u)^{1/n}) \prod_{k=1}^n (1 + k/\alpha)^{1/n}}{\prod_{k=1}^n ((n+k)/\alpha) + 1 + \beta(\alpha)/\alpha)^{1/n}}$$
$$= 2.$$

It follows that there is some $\alpha > -1$ such that $\prod_{k=1}^n \left(1 - y_k^{(\alpha,\beta(\alpha))}\right) = u$ and $\prod_{k=1}^n \left(1 + y_k^{(\alpha,\beta(\alpha))}\right) = v$. $\square$

PROOF OF LEMMA 3.2. Fix $s \geq 0$ and set for $t \geq 0$, $n \in \mathbb{N}$,

$$g_n(t) = \prod_{k=1}^n \left(\frac{k + (s+t)/2}{k+s}\right)^{k+s} \left(\frac{k+t}{k + (s+t)/2}\right)^{k+t} \left(\frac{n+k+2s}{n+k+s+t}\right)^{n+k+2s}.$$

Obviously, $g_n(s) = 1$. To see that $g_n(t) > 1$ for $t \neq s$ consider

$$h_n(t) = \log \frac{g_n(t)}{g_{n-1}(t)}$$
$$= \log\left[\frac{(n+s)^{n+s}(n+t)^{n+t}}{(n+(s+t)/2)^{2n+s+t}} \left(\frac{2n-1+2s}{2n-1+s+t}\right)^{2n-1+2s} \left(\frac{n+s+t}{n+2s}\right)^{n+2s} \right],$$

where $g_0(t)=1$. If $t>s$, then

$$\begin{aligned} h_n'(t) &= \frac{(s-t)(n-1)}{(n+s+t)(2n-1+s+t)} + \log\frac{2n+2t}{2n+s+t} \\ &> (t-s)\left(\frac{1-n}{(n+s+t)(2n-1+s+t)} + \frac{4n+3s+t}{2(2n+s+t)^2}\right) \\ &> 0, \end{aligned}$$

the first inequality following from the fact that $\log y > y-1-\frac{1}{2}(y-1)^2$ for $y>1$. Similarly, if $0\le t<s$, then $h_n'(t)<0$. As $h_n(s)=0$, it now follows that $h_n(t)>0$ for all $t\ne s$. Thus $g_n(t)=\exp(\sum_{k=1}^n h_k(t))>1$ for $t\ne s$. □

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INSTITUT FÜR STATISTIK
RWTH AACHEN
D-52056 AACHEN
GERMANY
E-MAIL: imhof@stochastik.rwth-aachen.de