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A delimitation of the support of optimal designs for Kiefer's ϕ_p-class of criteria

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ABSTRACT

The paper extends the result of Harman and Pronzato [Harman, R., Pronzato, L., 2007. Improvements on removing non-optimal support points in *D*-optimum design algorithms. Statistics & Probability Letters 77, 90–94], which corresponds to $p = 0$, to all strictly concave criteria in Kiefer's ϕ_p-class. We show that, for any given design measure ξ, any support point $\mathbf{x}_*$ of a ϕ_p-optimal design is such that the directional derivative of ϕ_p at ξ in the direction of the delta measure at $\mathbf{x}_*$ is larger than some bound $h_p[\xi]$ which is easily computed.

1. Introduction and motivation

For $\mathscr{X}$ a compact subset of $\mathbb{R}^m$, denote by Ξ the set of design measures (i.e., probability measures) on $\mathscr{X}$ and by $\mathbf{M}(\xi)$ the information matrix

$$\mathbf{M}(\xi) = \int_{\mathscr{X}} \mathbf{x}\mathbf{x}^\top \, \xi(\mathrm{d}\mathbf{x}).$$

We suppose that there exists a nonsingular design on $\mathscr{X}$ (i.e., there exists a $\xi \in \Xi$ such that $\mathbf{M}(\xi)$ is nonsingular) and we denote by Ξ^+ the set of such designs. We consider an optimal design problem on $\mathscr{X}$ defined by the maximization of a design criterion $\phi(\xi) = \Phi[\mathbf{M}(\xi)]$ with respect to $\xi \in \Xi$. One may refer to Pukelsheim (1993, Chap. 5) for a presentation of desirable properties that make a criterion $\Phi(\cdot)$ appropriate to measure the information provided by ξ. Here we shall focus our attention on design criteria that correspond to the ϕ_p-class considered by Kiefer (1974). More precisely, we consider the positively homogeneous form of such criteria and, for any $\mathbf{M} \in \mathbb{M}$, the set of symmetric non-negative definite $m \times m$ matrices, we denote

$$\Phi_p^+(\mathbf{M}) = \left[\frac{1}{m}\,\mathrm{tr}(\mathbf{M}^{-p})\right]^{-1/p}, \tag{1}$$

with the continuous extension $\Phi_p^+(\mathbf{M}) = 0$ when $\mathbf{M}$ is singular and $p \geq 0$. A design measure ξ_p^* that maximizes $\phi_p(\xi) = \Phi_p^+[\mathbf{M}(\xi)]$ will be said ϕ_p-optimal. Note that when $p \neq 0$ the maximization of $\Phi_p^+(\mathbf{M})$ is equivalent to the minimization of $\left[\mathrm{tr}(\mathbf{M}^{-p})\right]^{1/p}$, and thus to the minimization of $\mathrm{tr}(\mathbf{M}^{-p})$ when p is positive. A classical example is A-optimal design,

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which corresponds to $p = 1$. Taking the limit of $\Phi_p^+(\cdot)$ when p tends to zero, we obtain $\Phi_0^+(\mathbf{M}) = [\det(\mathbf{M})]^{1/m}$, which corresponds to D-optimal design. The limit when p tends to infinity gives $\Phi_\infty(\mathbf{M}) = \lambda_{\min}(\mathbf{M})$, the minimum eigenvalue of $\mathbf{M}$, and corresponds to E-optimal design. Some basic properties of ϕ_p-optimal designs are briefly recalled in Section 2.

Classical algorithms for optimal design usually apply to situations where $\mathscr{X}$ is a finite set. The performance of the algorithm (in particular, its execution time for a given required precision on $\phi(\cdot)$) then heavily depends on the number k of elements in $\mathscr{X}$. The case of D-optimal design has retained much attention, see, for instance, Ahipasaoglu et al. (2008), Todd and Yildirim (2007), Yu (2010) and Yu (2011). Harman and Pronzato (2007) show how any nonsingular design on $\mathscr{X}$ yields a simple inequality that must be satisfied by the support points of a D-optimal design ξ_0^*. Whatever the iterative method used for the construction of ξ_0^*, this delimitation of the support of ξ_0^* permits one to reduce the cardinality of $\mathscr{X}$ along the iterations, with the inequality becoming more stringent when approaching the optimum, hence producing a significant acceleration of the algorithm. Put in other words, the delimitation of the support of an optimal design facilitates the optimization by focusing the search on the useful part of the design space $\mathscr{X}$. The objective of the paper is to extend the results in Harman and Pronzato (2007) to the ϕ_p-class (1) of design criteria. The condition obtained does not tell us what the optimum support is, but indicates where it cannot be.

The paper is organized as follows. Section 2 recalls the main properties of ϕ_p-optimal design that are useful for the rest of the paper. The main result is derived in Section 3 and illustrative examples are given in Section 4. Finally, Section 5 concludes and indicates some possible extensions.

2. Some basic properties of ϕ_p-optimal designs

The criteria $\Phi_p^+(\cdot)$ defined by (1) satisfy $\Phi_p^+(\mathbf{I}_m) = 1$ for $\mathbf{I}_m$ the m-dimensional identity matrix and $\Phi_p^+(a\mathbf{M}) = a\,\Phi_p^+(\mathbf{M})$ for any $a > 0$ and any $\mathbf{M} \in \mathbb{M}$. Note that, from Caratheodory's theorem, a finitely-supported optimal design always exists, with $m(m+1)/2$ support points at most. We also have the following properties.

Lemma 1. *For any $p \in (-1, \infty)$, the criterion $\Phi_p^+(\cdot)$ satisfies the following:*

(i) *$\Phi_p^+(\cdot)$ is strictly concave on the set $\mathbb{M}^+$ of symmetric positive definite $m \times m$ matrices; it is strictly isotonic (it preserves Löwner ordering) on $\mathbb{M}$ for $p \in (-1, 0)$; that is, $\Phi_p^+(\mathbf{M}_2) > \Phi_p^+(\mathbf{M}_1)$ for all $\mathbf{M}_1$ and $\mathbf{M}_2$ in $\mathbb{M}$ such that $\mathbf{M}_2 - \mathbf{M}_1 \in \mathbb{M}$ and $\mathbf{M}_2 \neq \mathbf{M}_1$; it is strictly isotonic on $\mathbb{M}^+$ for $p \in [0, \infty)$.*
(ii) *Any ϕ_p-optimal design ξ_p^* is nonsingular.*
(iii) *The optimal matrix $\mathbf{M}_* = \mathbf{M}_*[p]$ is unique.*

Part (i) is proved in Pukelsheim (1993, Chap. 6). For $p \geq 0$, (ii) follows from the observation that $\Phi_p^+(\mathbf{M}) = 0$ when $\mathbf{M}$ is singular while there exists a nonsingular $\mathbf{M}(\xi)$ with $\Phi_p^+[\mathbf{M}(\xi)] > 0$; for $p \in (-1, 0)$, the statement is proved in Pukelsheim (1993, Sect. 7.13) through the use of polar information functions. Part (iii) is a direct consequence of (i) and (ii): since an optimal design matrix $\mathbf{M}_*$ is nonsingular, the strict concavity of $\Phi_p^+(\cdot)$ at $\mathbf{M}_*$ implies that $\mathbf{M}_*$ is unique. Note that this does not imply that the optimal design measure ξ_p^* maximizing $\phi_p(\xi)$ is unique.

We shall only consider values of p in $(-1, \infty)$ and, from Lemma 1-(ii), we can thus restrict our attention to matrices $\mathbf{M}$ in $\mathbb{M}^+$. $\Phi_p^+(\cdot)$ is differentiable at any $\mathbf{M} \in \mathbb{M}^+$, with gradient

$$\nabla\Phi_p^+(\mathbf{M}) = \frac{1}{m}\,[\Phi_p^+(\mathbf{M})]^{p+1}\,\mathbf{M}^{-(p+1)} = \frac{\Phi_p^+(\mathbf{M})}{\mathrm{tr}(\mathbf{M}^{-p})}\,\mathbf{M}^{-(p+1)}.$$

The directional derivative $F_{\phi_p}(\xi;\nu) = \lim_{\alpha\to 0^+}(1/\alpha)\{\phi_p[(1-\alpha)\xi + \alpha\nu] - \phi_p(\xi)\}$ is well defined and finite for any $\xi \in \Xi^+$ and any $\nu \in \Xi$, with

$$F_{\phi_p}(\xi;\nu) = \mathrm{tr}\{[\mathbf{M}(\nu) - \mathbf{M}(\xi)]\nabla\Phi_p^+[\mathbf{M}(\xi)]\} = \phi_p(\xi)\left\{\frac{\int_{\mathscr{X}} \mathbf{x}^\top\mathbf{M}^{-(p+1)}(\xi)\mathbf{x}\,\nu(d\mathbf{x})}{\mathrm{tr}[\mathbf{M}^{-p}(\xi)]} - 1\right\}.$$

We shall denote by $F_{\phi_p}(\xi,\mathbf{x}) = F_{\phi_p}(\xi;\delta_{\mathbf{x}})$ the directional derivative of $\phi_p(\cdot)$ at ξ in the direction of the delta measure at $\mathbf{x}$,

$$F_{\phi_p}(\xi,\mathbf{x}) = \phi_p(\xi)\left\{\frac{\mathbf{x}^\top\mathbf{M}^{-(p+1)}(\xi)\mathbf{x}}{\mathrm{tr}[\mathbf{M}^{-p}(\xi)]} - 1\right\}. \tag{2}$$

The following theorem, which relies on the concavity and differentiability of $\Phi_p^+(\cdot)$, is a classical result in optimal design theory, see, e.g., Kiefer (1974) and Pukelsheim (1993, Chap. 7).

Theorem 1 (*Equivalence Theorem*)**.** *For any $p \in (-1, \infty)$, the following statements are equivalent:*

(i) *ξ_p^* is ϕ_p-optimal.*
(ii) *$\mathbf{x}^\top\mathbf{M}^{-(p+1)}(\xi_p^*)\mathbf{x} \leq \mathrm{tr}[\mathbf{M}^{-p}(\xi_p^*)]$ for all $\mathbf{x} \in \mathscr{X}$.*
(iii) *ξ_p^* minimizes $\max_{\mathbf{x}\in\mathscr{X}} F_{\phi_p}(\xi,\mathbf{x})$ with respect to $\xi \in \Xi^+$.*

Moreover, the inequality of (ii) holds with equality for every support point $\mathbf{x} = \mathbf{x}_*$ of ξ_p^*.