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# A delimitation of the support of optimal designs for Kiefer's $\phi_p$ -class of criteria

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## Abstract

The paper extends the result of Harman and Pronzato [Stat. & Prob. Lett., 77:90–94, 2007], which corresponds to  $p = 0$ , to all strictly concave criteria in Kiefer's  $\phi_p$ -class. Let  $\xi$  be any design on a compact set  $\mathcal{X} \subset \mathbb{R}^m$  with a nonsingular information matrix  $\mathbf{M}(\xi)$ , and let  $\delta$  be the maximum of the directional derivative  $F_{\phi_p}(\xi, \mathbf{x})$  over all  $\mathbf{x} \in \mathcal{X}$ . We show that any support point  $\mathbf{x}_*$  of a  $\phi_p$ -optimal design satisfies the inequality  $F_{\phi_p}(\xi, \mathbf{x}_*) \geq h_p[\mathbf{M}(\xi), \delta]$ , where the bound  $h_p[\mathbf{M}(\xi), \delta]$  is easily computed: it requires the determination of the unique root of a simple univariate equation (polynomial when  $p$  is integer) in a given interval. The construction can be used to accelerate algorithms for  $\phi_p$ -optimal design and is illustrated on an example with  $A$ -optimal design.

**keywords** Approximate design; optimum design; support points; design algorithm

**MSC** 62K05; 90C46

## 1 Introduction and motivation

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

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

We suppose that there exists a nonsingular design on  $\mathcal{X}$  (i.e., there exists a  $\xi \in \Xi$  such that  $\mathbf{M}(\xi)$  is nonsingular) and we denote by  $\Xi^+$  the set of such designs. We consider an optimal

design problem on  $\mathcal{X}$  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  $\xi$ . Here we shall focus our attention on design criteria that correspond to the  $\phi_p$ -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

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

with the continuous extension  $\Phi_p^+(\mathbf{M}) = 0$  when  $\mathbf{M}$  is singular and  $p \geq 0$ . A design measure  $\xi_p^*$  that maximizes  $\phi_p(\xi) = \Phi_p^+[\mathbf{M}(\xi)]$  will be said  $\phi_p$ -optimal. Note that when  $p \neq 0$  the maximization of  $\Phi_p^+(\mathbf{M})$  is equivalent to the minimization of  $[\text{tr}(\mathbf{M}^{-p})]^{1/p}$ , and thus to the minimization of  $\text{tr}(\mathbf{M}^{-p})$  when  $p$  is positive. A classical example is  $A$ -optimal design, 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  $\phi_p$ -optimal designs are briefly recalled in Sect. 2.

Classical algorithms for optimal design usually apply to situations where  $\mathcal{X}$  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  $\mathcal{X}$ . 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  $\mathcal{X}$  yields a simple inequality that must be satisfied by the support points of a  $D$ -optimal design  $\xi_0^*$ . Whatever the iterative method used for the construction of  $\xi_0^*$ , this delimitation of the support of  $\xi_0^*$  permits to reduce the cardinality of  $\mathcal{X}$  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 focussing the search on the useful part of the design space  $\mathcal{X}$ . The objective of the paper is to extend the results in Harman and Pronzato (2007) to the  $\phi_p$ -class (1) of design criteria. The condition obtained does not tell what the optimum support is, but indicates where it cannot be.

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

## 2 Some basic properties of $\phi_p$ -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 on  $\mathbb{M}$  for  $p \in (-1, 0)$  and strictly isotonic on  $\mathbb{M}^+$  for  $p \in [0, \infty)$ .
- (ii) Any  $\phi_p$ -optimal design  $\xi_p^*$  is nonsingular.
- (iii) The optimal matrix  $\mathbf{M}_* = \mathbf{M}_*[p]$  is unique.

Part (i) is proved in Pukelsheim (1993, Chap. 6) and the proof of (ii) is given in Appendix; (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  $\xi_p^*$  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

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

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

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

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  $\xi$  in the direction of the delta measure at  $\mathbf{x}$ ,

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

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)  $\xi_p^*$  is  $\phi_p$ -optimal.

(ii)  $\mathbf{x}^\top \mathbf{M}^{-(p+1)}(\xi_p^*) \mathbf{x} \leq \text{tr}[\mathbf{M}^{-p}(\xi_p^*)]$  for all  $\mathbf{x} \in \mathcal{X}$ .

(iii)  $\xi_p^*$  minimizes  $\max_{\mathbf{x} \in \mathcal{X}} F_{\phi_p}(\xi, \mathbf{x})$  with respect to  $\xi \in \Xi^+$ .

### 3 A necessary condition for support points of $\phi_p$ -optimal designs

#### 3.1 A lower bound on $\mathbf{x}^\top \mathbf{M}^{-(p+1)} \mathbf{x}$ for the support points of an optimal design

Take any  $p \in (-1, \infty)$  and any  $\xi \in \Xi^+$ . We shall omit the dependence in  $\xi$  when there is no ambiguity and simply write  $\mathbf{M} = \mathbf{M}(\xi)$ ,  $\phi_p = \phi_p(\xi)$ . We shall also denote

$$t = t(\xi, p) = \text{tr}[\mathbf{M}^{-p}], \quad t_* = t_*(p) = \text{tr}(\mathbf{M}_*^{-p}),$$

with  $\mathbf{M}_*$  the optimal matrix satisfying  $\phi_p^* = \Phi_p^+(\mathbf{M}_*) = \max_{\nu \in \Xi} \Phi_p^+[\mathbf{M}(\nu)]$ . Define

$$\epsilon = \epsilon(\xi, p) = \max_{\mathbf{x} \in \mathcal{X}} \{\mathbf{x}^\top \mathbf{M}^{-(p+1)} \mathbf{x}\} - t. \quad (3)$$

The concavity of  $\Phi_p^+(\cdot)$  implies that  $\phi_p \leq \phi_p^* \leq \phi_p + F_{\phi_p}(\xi; \xi_p^*) \leq \phi_p(\xi) + \max_{x \in \mathcal{X}} F_{\phi_p}(\xi, \mathbf{x})$ , with  $\xi_p^*$  denoting a  $\phi_p$ -optimal design measure; that is,

$$\phi_p \leq \phi_p^* \leq \phi_p(1 + \epsilon/t), \quad (4)$$

see (2).

Since  $\mathbf{x}^\top \mathbf{M}^{-(p+1)} \mathbf{x} \leq t + \epsilon$  for all  $\mathbf{x} \in \mathcal{X}$ , see (3), we have

$$\text{tr}[\mathbf{M}_* \mathbf{M}^{-(p+1)}] \leq t + \epsilon. \quad (5)$$

On the other hand, the optimality of  $\xi_p^*$  implies (see Th. 1-(ii))

$$\text{tr}[\mathbf{M} \mathbf{M}_*^{-(p+1)}] \leq t_*. \quad (6)$$

Moreover, any support point  $\mathbf{x}_*$  of  $\xi_p^*$  satisfies  $\mathbf{x}_*^\top \mathbf{M}_*^{-(p+1)} \mathbf{x}_* = t_*$ . We use a construction similar to that in Harman and Pronzato (2007) and define  $\mathbf{H} = \mathbf{H}(\xi, p) = \mathbf{M}^{-(p+1)/2} \mathbf{M}_*^{p+1} \mathbf{M}^{-(p+1)/2}$ . Then we can write

$$\mathbf{x}_*^\top \mathbf{M}^{-(p+1)} \mathbf{x}_* = \mathbf{x}_*^\top \mathbf{M}^{-(p+1)/2} \mathbf{H}^{-1/2} \mathbf{H} \mathbf{H}^{-1/2} \mathbf{M}^{-(p+1)/2} \mathbf{x}_* \geq \lambda_1 \mathbf{x}_*^\top \mathbf{M}_*^{-(p+1)} \mathbf{x}_* = \lambda_1 t_*,$$

with  $\lambda_1 = \lambda_1(\xi, \xi_p^*, p) = \lambda_{\min}(\mathbf{H})$ , the minimum eigenvalue of  $\mathbf{H}$ . Notice that  $\lambda_1 > 0$ .  $\lambda_1$  depends on  $\mathbf{M}_*$  which is unknown. Below we shall construct a lower bound  $\underline{\lambda}_1$  on  $\lambda_1$  and thus obtain a necessary condition for support points  $\mathbf{x}_*$  of  $\xi_p^*$ , in the form:

$$\mathbf{x}_*^\top \mathbf{M}^{-(p+1)} \mathbf{x}_* \geq \underline{\lambda}_1 t_*. \quad (7)$$

When  $p = 0$  ( $D$ -optimal design), we have  $t = t_* = m$ , and this necessary condition is simply

$$\mathbf{x}_*^\top \mathbf{M}^{-1} \mathbf{x}_* \geq \underline{\lambda}_1 m \quad (p = 0); \quad (8)$$

it corresponds to the case treated in Harman and Pronzato (2007). When  $p \neq 0$ ,  $t_*$  is usually unknown and we shall use

$$\mathbf{x}_*^\top \mathbf{M}^{-(p+1)} \mathbf{x}_* \geq \underline{\lambda}_1 t (1 + \epsilon/t)^{-p} \quad \text{for } p > 0, \quad (9)$$

$$\mathbf{x}_*^\top \mathbf{M}^{-(p+1)} \mathbf{x}_* \geq \underline{\lambda}_1 t \quad \text{for } -1 < p < 0, \quad (10)$$

see (4) and the definitions of  $t, t_*, \phi_p, \phi_p^*$ . Next section is devoted to the construction of the lower bound  $\underline{\lambda}_1$ , using the inequalities (5) and (6).

### 3.2 Construction of the lower bound $\underline{\lambda}_1$

The inequality (5) can be rewritten as  $\text{tr}(\mathbf{H}^{1/(p+1)} \mathbf{M}^{-p}) \leq t + \epsilon$  and (6) can be rewritten as  $\text{tr}(\mathbf{H}^{-1} \mathbf{M}^{-p}) \leq t_*$ . Consider the spectral decomposition  $\mathbf{H} = \mathbf{S} \mathbf{\Lambda} \mathbf{S}^\top$ , with  $\mathbf{S} \mathbf{S}^\top = \mathbf{S}^\top \mathbf{S} = \mathbf{I}_m$  and  $\mathbf{\Lambda}$  the diagonal matrix whose diagonal elements are the eigenvalues  $\lambda_i$  of  $\mathbf{H}$  sorted by increasing values. Denote  $\mathbf{B} = \mathbf{S}^\top \mathbf{M}^{-p} \mathbf{S}$  and  $b_i = \{\mathbf{B}\}_{ii}$  its diagonal elements,  $i = 1, \dots, m$ .  $\mathbf{B}$  has the same set of eigenvalues as  $\mathbf{M}^{-p}$  and

$$0 < \underline{b}_1 = \lambda_{\min}(\mathbf{M}^{-p}) \leq b_i \leq \lambda_{\max}(\mathbf{M}^{-p}), \quad i = 1, \dots, m, \quad (11)$$

see, e.g., Magnus and Neudecker (1999, p. 211). We then obtain that (5) and (6) are respectively equivalent to

$$\begin{aligned} \sum_{i=1}^m b_i \lambda_i^{1/(p+1)} &\leq t + \epsilon, \\ \sum_{i=1}^m b_i / \lambda_i &\leq t_*. \end{aligned} \quad (12)$$

**Remark 1** Inequality (12) implies that  $\underline{\lambda}_1 \geq b_1/t_* \geq \underline{b}_1/t_*$ . When plugged in (7), it gives  $\mathbf{x}_*^\top \mathbf{M}^{-(p+1)} \mathbf{x}_* \geq \underline{b}_1$ . Although this bound is rather loose for  $m \geq 2$ , it cannot be improved when  $m = 1$ . Indeed,  $m = 1$  implies  $\underline{b}_1 = b_1 = t$  and the inequality  $\mathbf{x}_*^\top \mathbf{M}^{-(q+1)} \mathbf{x}_* \geq t$  is the tightest we can obtain, see Th. 1-(ii). In the following we shall suppose that  $m \geq 2$ .

Denote  $\omega_i = \lambda_i^{1/(p+1)}$  for  $i = 1, \dots, m \geq 2$ . The determination of  $\underline{\lambda}_1$  amounts to the solution of the following optimization problem: minimize  $\omega_1$  with respect to  $\omega = (\omega_1, \dots, \omega_m)^\top$  under the constraints  $0 \leq \omega_1 \leq \omega_2 \leq \dots \leq \omega_m$ ,  $\sum_{i=1}^m b_i \omega_i \leq t + \epsilon$  and  $\sum_{i=1}^m b_i / \omega_i^{p+1} \leq t_*$ . This is a convex problem, with Lagrangian

$$L(\omega, \mu_1, \mu_2) = \omega_1 + \mu_1 \left( \sum_{i=1}^m b_i \omega_i - t - \epsilon \right) + \mu_2 \left( \sum_{i=1}^m b_i / \omega_i^{p+1} - t_* \right).$$

Its stationarity with respect to  $\omega$  indicates that the optimal solution satisfies  $\omega_i = \omega_2$  for all  $i \geq 2$ . Since  $\sum_{i=1}^m b_i = \text{tr}(\mathbf{M}^{-p}) = t$ , from the Kuhn-Tucker conditions we obtain

$$\begin{aligned} b_1 \omega_1 + (t - b_1) \omega_2 &= t + \epsilon, \\ b_1 / \omega_1^{p+1} + (t - b_1) / \omega_2^{p+1} &= t_*, \end{aligned}$$

or equivalently

$$\alpha \omega_1 + (1 - \alpha) \omega_2 = 1 + \beta, \quad (13)$$

$$\alpha / \omega_1^{p+1} + (1 - \alpha) / \omega_2^{p+1} = \gamma_*, \quad (14)$$

where  $\alpha = b_1/t$ ,  $\beta = \epsilon/t \geq 0$  and  $\gamma_* = t^*/t$ .

When  $p = 0$  ( $D$ -optimal design), then  $\alpha = 1/m$ ,  $\gamma_* = 1$  and (13), (14) can be directly solved for  $\omega_1, \omega_2$ , yielding  $\underline{\lambda}_1 = \omega_1$  to be used in (8), see Harman and Pronzato (2007). However, when  $p \neq 0$ ,  $\alpha$  depends on  $\mathbf{M}_*$  and  $\gamma_*$  depends on  $t_*$  and are thus usually unknown. We must then determine the lowest value of  $\omega_1 \leq \omega_2$  satisfying (13), (14) given the information available on  $\alpha$  and  $\gamma_*$ ; that is, respectively, (11) which gives  $1 > \alpha \geq \underline{b}_1/t = \lambda_{\min}(\mathbf{M}^{-p})/\text{tr}(\mathbf{M}^{-p})$ , and (4) which implies that  $\gamma_*$  satisfies

$$\gamma_* \in [(1 + \beta)^{-p}, 1] \quad \text{if } p \geq 0, \quad (15)$$

$$\gamma_* \in [1, (1 + \beta)^{-p}] \quad \text{if } p \leq 0. \quad (16)$$

The solution to this problem is given in appendix and yields the main result of the paper.

**Theorem 2** For any  $p \in (-1, \infty)$  and any design  $\xi \in \Xi^+$ , any point  $\mathbf{x}_* \in \mathcal{X}$  such that

$$\mathbf{x}_*^\top \mathbf{M}^{-(p+1)}(\xi) \mathbf{x}_* < C(\xi, p) = \omega_1^{p+1} B(t, \epsilon) \quad (17)$$

cannot be support point of a  $\phi_p$ -optimal design measure  $\xi_p^*$ , where we denoted  $t = \text{tr}[\mathbf{M}^{-p}(\xi)]$ ,  $\epsilon = \max_{\mathbf{x} \in \mathcal{X}} \mathbf{x}^\top \mathbf{M}^{-(p+1)}(\xi) \mathbf{x} - t$ ,  $B(t, \epsilon) = t \min\{1, (1 + \epsilon/t)^{-p}\}$ , and where  $\omega_1$  is the unique solution for  $\theta$  in the interval  $((\alpha/\gamma)^{1/(p+1)}, (1/\gamma)^{1/(p+1)})$  of the equation

$$F(\theta; \alpha, \epsilon, t, \gamma, p) = \frac{\alpha}{\theta^{p+1}} + \frac{(1 - \alpha)^{p+2}}{(1 + \epsilon/t - \alpha\theta)^{p+1}} - \gamma = 0 \quad (18)$$

with  $\alpha = \lambda_{\min}[\mathbf{M}^{-p}(\xi)]/\text{tr}[\mathbf{M}^{-p}(\xi)]$  and  $\gamma = \max\{1, (1 + \epsilon/t)^{-p}\}$ .

In the special case when  $t_* = \text{tr}[\mathbf{M}^{-p}(\xi_p^*)]$  is known (thus in particular if  $p = 0$ ), one can take  $B(t, \epsilon) = t_*$  and  $\gamma = \gamma_* = t^*/t$  in (17), (18).

**Remark 2**

1. When  $p$  is integer,  $F(\theta; \alpha, \epsilon, t, \gamma, p) = 0$  is a polynomial equation in  $\theta$  of degree  $2(p+1)$ .
2. From the definition (3) of  $\epsilon = \epsilon(\xi, p)$ ,  $\delta = \max_{\mathbf{x} \in \mathcal{X}} F_{\phi_p}(\xi, \mathbf{x}) = \epsilon \phi_p(\xi)/t$ , see (2), and (17) is equivalent to  $F_{\phi_p}(\xi, \mathbf{x}_*) < h_p[\mathbf{M}(\xi), \delta] = \phi_p(\xi) [C(\xi, p)/t - 1]$ . Note that  $C(\xi, p) \leq t$ , so that all points  $\mathbf{x}$  such that  $F_{\phi_p}(\xi, \mathbf{x}) \geq 0$  are potential support points of  $\xi_p^*$ .
3. Suppose  $p > 0$  with  $t_*$  unknown and  $\epsilon \rightarrow \infty$ ; then,  $B(t, \epsilon) \rightarrow 0$ , so that  $C(\xi, p) \rightarrow 0$  and the condition (17) brings no information on the support of  $\xi_p^*$ . The same is true when  $p < 0$  with  $t_*$  unknown and  $\epsilon \rightarrow \infty$ :  $\gamma \rightarrow \infty$ , so that  $\omega_1 \rightarrow 0$  and again  $C(\xi, p) \rightarrow 0$ . Suppose now that  $t_*$  is known. Then,  $C(\xi, p) = t_* \omega_1^{p+1} \in (\lambda_{\min}[\mathbf{M}^{-p}(\xi)], \text{tr}[\mathbf{M}^{-p}(\xi)])$  and  $\omega_1^{p+1} \rightarrow \alpha/\gamma_* = \lambda_{\min}[\mathbf{M}^{-p}(\xi)]/t_*$  as  $\epsilon \rightarrow \infty$ , see (18), so that  $C(\xi, p) \rightarrow \underline{b}_1 = \lambda_{\min}[\mathbf{M}^{-p}(\xi)]$  and we recover the same bound as in Remark 1.
4. Using a construction similar to that in Harman and Pronzato (2007, Th. 3), one can show that the bound (17) with  $B(t, \epsilon) = t_*$  and  $\gamma = t^*/t$  gives the tightest necessary condition for support points: for any  $m \geq 2$ , any  $\epsilon > 0$  and any  $\delta > 0$ , one can exhibit an example with a design space  $\mathcal{X}$ , a design measure  $\xi$  such that  $\max_{\mathbf{x} \in \mathcal{X}} \{\mathbf{x}^\top \mathbf{M}^{-(p+1)} \mathbf{x}\} - t = \epsilon$ , and an optimal design  $\xi_p^*$  with support point  $\mathbf{x}_*$  such that  $\mathbf{x}_*^\top \mathbf{M}^{-(p+1)} \mathbf{x}_* < \omega_1^{p+1} t_* + \delta$  (with  $\mathbf{M}$  and  $\mathbf{M}_*$  diagonal and  $\mathbf{H}$  having eigenvalues  $\lambda_1 < \lambda_2 = \dots = \lambda_m$ ).

## 4 Examples

**Example 1.** Consider the linear regression model with  $\mathbf{x} = \mathbf{x}(s) = (1, s, s^2)^\top$ ,  $s \in [-1, 1]$  ( $m = 3$ ). For any  $p \in (-1, \infty)$ , the  $\phi_p$ -optimal design on  $[-1, 1]$  is unique and is supported at the three points  $\{-1, 0, 1\}$ . For symmetry reasons, it corresponds to

$$\xi_\tau = \tau \delta_{-1} + (1 - 2\tau) \delta_0 + \tau \delta_1$$

for some particular  $\tau^* = \tau^*(p)$ , with  $\tau^*(-1/2) = 0.45$ ,  $\tau^*(0) = 1/3$  ( $D$ -optimal design),  $\tau^*(1) = 1/4$  ( $A$ -optimal design) and, in the limit  $p \rightarrow \infty$ ,  $\tau^*(\infty) = 0.2$  ( $E$ -optimal design), see Fig. 2-left for a plot of  $\tau^*(p)$  for  $p \in [-1/2, 1]$ . Here,  $\delta_s$  denotes the Dirac delta measure at  $s$ .

To illustrate the impact of not knowing  $t_*$  on the construction of  $\omega_1^{p+1}$  through the solution of (18), we take  $p = 1$  and compute  $\omega_1^{p+1}$  for the cases  $\gamma = 1$  ( $t_*$  unknown) and  $\gamma = t^*/t$  ( $t_*$  known) for different designs  $\xi_\tau$ ,  $\tau \in [\tau^*(1) - 1/16, \tau^*(1) + 1/16]$ . Figure 1 shows that the value obtained for  $t_*$  unknown (solid line) is not much worse, i.e., smaller, than the value for  $t_*$  known (dashed line). Note that considering different designs  $\xi_\tau$  with  $\tau \neq \tau^*(p)$  is equivalent to considering different  $\epsilon$  given by (3), with  $\epsilon$  being approximately linear in  $|\tau - \tau^*(p)|$  for the range of values of  $\tau$  considered.



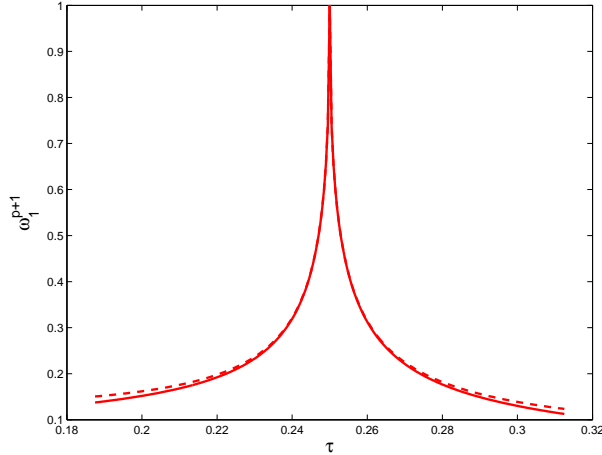


Figure 1: Value of  $\omega_1^{p+1}$  for different designs  $\xi_\tau$ ,  $\tau \in [3/16, 5/16]$  ( $p = 1$ ,  $t_*$  unknown in *solid line*,  $t_*$  known in *dashed line*).

The marginal deterioration of the bound (17) due to the ignorance of  $t_*$  when  $\epsilon$  is small enough is further illustrated by Fig. 2. Here, we set  $\epsilon$  at some fixed value (the values  $\epsilon = 0.1$  and  $\epsilon = 1$  are considered), and for values of  $p$  in the range  $[-1/2, 1]$  we compute  $\tau(p, \epsilon)$  such that  $\max_{s \in [-1, 1]} \mathbf{x}^\top(s) \mathbf{M}^{-(p+1)}(\xi_\tau) \mathbf{x}(s) = \text{tr}[\mathbf{M}^{-p}(\xi_\tau)] + \epsilon$ . The values of  $\tau^*(p)$  and  $\tau(p, 0.1)$  are shown in Fig. 2-left, in solid and dashed lines respectively. Then, for each  $p$  and associated design  $\xi_{\tau(p, \epsilon)}$  we compute the bound  $C(\xi_{\tau(p, \epsilon)}, p)$  of (17) in the two situations  $t_*$  unknown and  $t_*$  known; see the plots in Fig. 2-right. Note that bound for  $t_*$  unknown (solid line) remains near the bound for  $t_*$  known (dashed line) when  $\epsilon = 0.1$ ; the situation deteriorates for larger  $\epsilon$  but the two bounds get close as  $p$  approaches 0 and exactly coincide at  $p = 0$  (since then  $t = t_* = m$ ).

**Example 2.** Take now the complete product-type interaction model  $\mathbf{x}(\mathbf{s}) = \mathbf{x}(s_1) \otimes \mathbf{x}(s_2)$ ,  $\mathbf{s} = (s_1, s_2)$ , with  $\otimes$  denoting tensor product and  $\mathbf{x}(s_i) = (1, s_i, s_i^2)^\top$ ,  $s_i \in [-1, 1]$ , for  $i = 1, 2$  ( $m = 9$ ). The  $D$ -optimal (respectively  $A$ -optimal) design for this problem is the cross product of two  $D$ -optimal designs (resp.  $A$ -optimal designs) for one single factor, i.e., it corresponds to the cross product of two designs  $\xi_\tau$  with  $\tau = 1/3$  (resp.  $\tau = 1/4$ ), see Schwabe (1996, Chap. 4 and 5). The optimal values of  $\phi_p$ ,  $p = 0, 1$ , are  $\phi_0^* = 16^{1/3}/9 \simeq 0.2800$  and  $\phi_1^* = 9/64 \simeq 0.1406$ .

We consider the iterative construction of optimal designs through the recursion

$$w_i^{k+1} = w_i^k \frac{[\mathbf{x}_i^\top \mathbf{M}^{-(p+1)}(\xi_k) \mathbf{x}_i]^a}{\sum_{i=1}^{N_k} [\mathbf{x}_i^\top \mathbf{M}^{-(p+1)}(\xi_k) \mathbf{x}_i]^a}, \quad (19)$$

where  $\xi_k$ , the design measure at iteration  $k$ , allocates mass  $w_i^k$  at the point  $\mathbf{x}_i$  present in  $\mathcal{X}$  at iteration  $k$ ,  $i = 1, \dots, N_k$ . The initial design space corresponds to a uniform grid for  $\mathbf{s}$ , with  $s_i$  varying from  $-1$  to  $1$  by steps of  $0.05$  (41 values),  $i = 1, 2$ , which gives  $N_0 = 1681$ . The initial

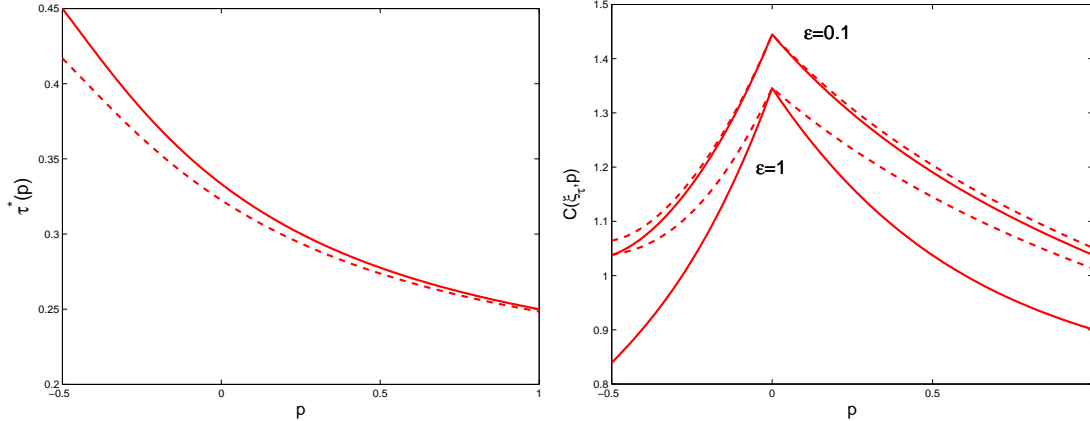


Figure 2: Left:  $\tau^*(p)$  such that  $\xi_{\tau^*(p)} = \xi_p^*$  is  $\phi_p$ -optimal for  $p$  (solid line) and  $\tau(p, \epsilon)$  such that  $\max_{s \in [-1, 1]} \mathbf{x}^\top(s) \mathbf{M}^{-(p+1)}(\xi_{\tau(p, \epsilon)}) \mathbf{x}(s) = \text{tr}[\mathbf{M}^{-p}(\xi_{\tau(p, \epsilon)})] + \epsilon$  ( $\epsilon = 0.1$ , dashed line). Right: bound  $C(\xi_{\tau(p, \epsilon)}, p)$  in (17) for the two cases  $t_*$  unknown (solid line) and  $t_*$  known (dashed line) for  $\epsilon = 0.1$  and  $\epsilon = 1$ .

design  $\xi_0$  is the uniform measure on those 1681 points. We take  $a = 1$  for  $D$ -optimal design ( $p = 0$ ) and  $a = 1/2$  for  $A$ -optimal design ( $p = 1$ ), which ensures monotonic convergence to the optimum, see Titterton (1976) and Pázman (1986) for  $D$ -optimal design and Torsney (1983) for  $A$ -optimal design; see also Fig. 3-left. Due to the convergence of  $\xi_k$  to the optimal design,  $\epsilon_k = \epsilon(\xi_k)$  given by (3) is decreasing with  $k$ , see Fig. 3-right.

We use inequality (17) to reduce the cardinality  $N_k$  of  $\mathcal{X}$  when possible: any point that violates (17) cannot be a support point of the optimal measure and is removed from  $\mathcal{X}$ . Here we simply set its mass to zero and rescale the weights of remaining point so that they sum to one, but more sophisticated reallocation rules can be used, see Harman and Pronzato (2007).  $N_k$  thus decreases with  $k$ , rendering the iterations (19) simpler and simpler as  $k$  increases. Figure 4 shows the evolution of  $N_k$  with  $k$ , both for  $D$ -optimal and  $A$ -optimal designs. The decrease of  $N_k$  is slower for the latter, the bound  $C(\xi, p)$  in (17) being more pessimistic, see Fig. 2-right, and  $\epsilon$  being larger, see Fig. 3-right. Note that the cancelation of points does not hamper the convergence of (19) since (17) is used a finite number of times only (obviously bounded by  $N_0$ ) — the heuristic rule used to reallocate weights of points that are removed may, however, impact monotonicity, although this is not the case in the present example, see Fig. 3-left.

## 5 Possible extensions and conclusions

Multivariate regression and Bayesian optimal design involve information matrices that can be expressed as  $\mathbf{M}(\xi) = \int_{\mathcal{X}} \mathcal{M}(\mathbf{x}) \xi(d\mathbf{x})$  with  $\mathcal{M}(\mathbf{x}) \in \mathbb{M}$  having rank larger than one (we suppose that  $\mathcal{M}(\cdot)$  is measurable and that  $\{\mathcal{M}(\mathbf{x}), \mathbf{x} \in \mathcal{X}\}$  forms a compact subset of  $\mathbb{M}$ ). The results

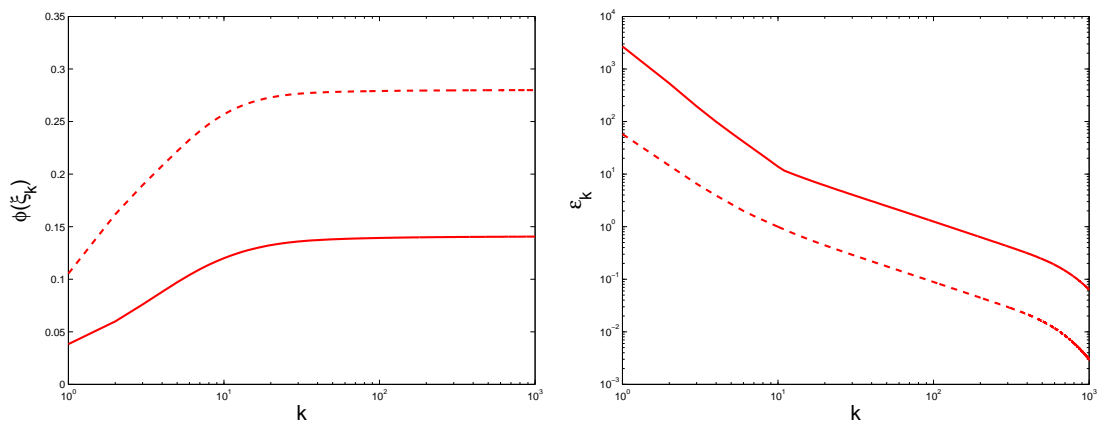


Figure 3:  $\phi(\xi_k)$  — left — and  $\epsilon_k = \epsilon(\xi_k)$  given by (3) — right — as functions of  $k$  for the recursion (19);  $D$ -optimal design is in *dashed line*,  $A$ -optimal design is in *solid line*.

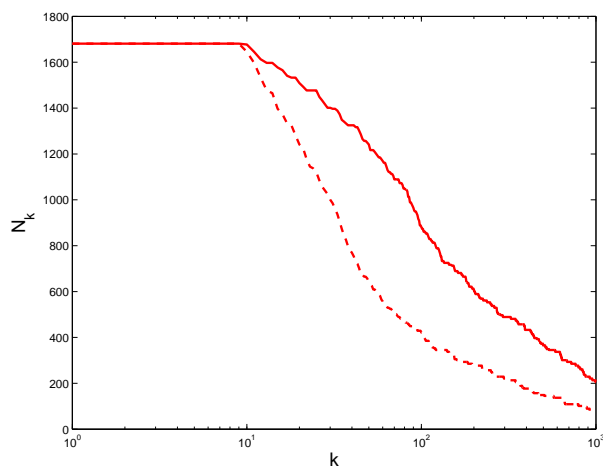


Figure 4:  $N_k$  as a function of  $k$  when using (17) to remove points from  $\mathcal{X}$ ; for  $D$ -optimal design (*dashed line*) and  $A$ -optimal design (*solid line*).

presented here can easily be extended to that situation, following the same lines as in Harman and Trnovská (2009) where the case  $p = 0$  is considered.

The  $E$ -optimality criterion  $\phi_E(\xi) = \Phi_E[\mathbf{M}(\xi)] = \lambda_{\min}[\mathbf{M}(\xi)]$  is not differentiable in general, but  $\Phi_E(\cdot)$  is differentiable at  $\mathbf{M}$  when  $\lambda_{\min}(\mathbf{M})$  has multiplicity one, with gradient  $\nabla\phi_E(\mathbf{M}) = \mathbf{v}\mathbf{v}^\top$  where  $\mathbf{v}$  denotes the eigenvector of unit length (unique up to a sign change) associated with  $\lambda_{\min}(\mathbf{M})$ . Although  $\phi_E(\xi)$  corresponds to the limit of  $\phi_p^+(\xi)$  as  $p$  tends to infinity, the results of Sect. 3 do not extend to this limiting situation, even in the differentiable case;  $E$ -optimality thus requires a special treatment and will be considered elsewhere.

The determination of a  $D$ -optimal design can be used for maximum-likelihood estimation in mixture models, see, e.g., Lindsay (1983) and Mallet (1986), and for the construction of the minimum-volume ellipsoid containing a compact set, see, e.g., Sibson (1972), Khachiyan and Todd (1993) and Khachiyan (1996). More generally, for any  $q \in (-1, \infty)$  the determination of the ellipsoid  $\mathcal{E}(\mathbf{A}) = \{\mathbf{z} \in \mathbb{R}^m : \mathbf{z}^\top \mathbf{A} \mathbf{z} \leq 1\}$ ,  $\mathbf{A} \in \mathbb{M}$ , containing the  $k$  points  $\mathbf{x}_1, \dots, \mathbf{x}_k$  of  $\mathbb{R}^m$  and such that  $\phi_q(\mathbf{A})$  is maximum is equivalent to the determination of a  $\phi_p$ -optimal design on  $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_k\}$  with  $p = -q/(1+q) \in (-1, \infty)$ , and the optimal matrix  $\mathbf{A}_*$  equals  $\mathbf{M}_*^{-(p+1)}/t_*$ ; see Pukelsheim (1993, Chap. 6). The delimitation of the support points of a  $\phi_p$ -optimal design can therefore also be used to accelerate the algorithmic construction of “ $\phi_q$ -optimal ellipsoids” containing compact sets.

In Sect. 4, we considered the suppression of points that cannot be support points of an optimal design in a multiplicative algorithm. When  $\mathcal{X}$  is not finite, or is finite but very large, it is advisable to use a vertex-direction or a vertex-exchange algorithm, see, e.g., Fedorov (1972), Wu (1978) and Böhning (1986). This requires the determination at each iteration, say iteration  $k$ , of a point  $\hat{\mathbf{x}}_k$  of  $\mathcal{X}$  that maximizes  $F_{\phi_p}(\xi_k, \mathbf{x})$  given by (2), at least approximately. Condition (17) of Theorem 2 can then be used to restrict the search for a suitable  $\hat{\mathbf{x}}_k$  in a domain that shrinks as  $k$  increases. Further developments are required to construct algorithms making an efficient use of (17) for the inclusion of new support points.

## Appendix

*Proof of Lemma 1-(ii).*

For  $p \geq 0$  the result 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  $p \in (-1, 0)$  we prove the result by contradiction. Take any  $\mathbf{M}_0 = \mathbf{M}(\xi_0)$  singular and consider its spectral decomposition in an orthonormal basis of eigenvectors  $\mathbf{v}_i$ ,  $i = 1, \dots, m$ :  $\mathbf{M}_0 = \sum_{i=1}^m \lambda_i \mathbf{v}_i \mathbf{v}_i^\top$ . Suppose that the eigenvalues  $\lambda_i$  are sorted by increasing values, so that  $\lambda_i = 0$  for  $i = 1, \dots, s$  when the eigenvalue 0 has multiplicity  $s$  (and  $\mathbf{M}_0$  has rank  $m - s$ ). Since

there exists a nonsingular design,  $\mathcal{X}$  spans  $\mathbb{R}^m$  and each eigenvector  $\mathbf{v}_i$ ,  $i = 1, \dots, s$ , can be written as  $\mathbf{v}_i = \gamma_i \int_{\mathcal{X} \cup (-\mathcal{X})} \mathbf{z} \mu_i(d\mathbf{z})$  for some  $\gamma_i > 0$ , where  $\mu_i(\cdot)$  is a probability measure on the compact set  $\mathcal{X} \cup (-\mathcal{X})$  (in fact, from Caratheodory's theorem, one may consider finitely supported measures only, with  $m + 1$  support points at most). Then,

$$\gamma_i^2 \int_{\mathcal{X} \cup (-\mathcal{X})} \mathbf{z} \mathbf{z}^\top \mu_i(d\mathbf{z}) - \mathbf{v}_i \mathbf{v}_i^\top = \int_{\mathcal{X} \cup (-\mathcal{X})} (\gamma_i \mathbf{z} - \mathbf{v}_i)(\gamma_i \mathbf{z} - \mathbf{v}_i)^\top \mu_i(d\mathbf{z}),$$

which is non-negative definite. Denote  $\mu(d\mathbf{z}) = [\sum_{i=1}^s \gamma_i^2 \mu_i(d\mathbf{z})] / (\sum_{i=1}^s \gamma_i^2)$ , which defines a probability measure on  $\mathcal{X} \cup (-\mathcal{X})$ . We thus obtain that, for any  $\alpha \in (0, 1)$ , the matrix

$$\left[ (1 - \alpha) \mathbf{M}_0 + \alpha \int_{\mathcal{X} \cup (-\mathcal{X})} \mathbf{z} \mathbf{z}^\top \mu(d\mathbf{z}) \right] - \left[ (1 - \alpha) \mathbf{M}_0 + \alpha \frac{\sum_{i=1}^s \mathbf{v}_i \mathbf{v}_i^\top}{\sum_{i=1}^s \gamma_i^2} \right]$$

is non-negative definite. Now,  $\int_{\mathcal{X} \cup (-\mathcal{X})} \mathbf{z} \mathbf{z}^\top \mu(d\mathbf{z})$  can be written as  $\int_{\mathcal{X}} \mathbf{x} \mathbf{x}^\top \tilde{\mu}(d\mathbf{x})$ , where  $\tilde{\mu}(\mathcal{A}) = \mu(\mathcal{A}) + \mu(-\mathcal{A})$  for any measurable set  $\mathcal{A} \subset \mathcal{X}$ , and  $\tilde{\mu}(\cdot)$  is thus a design measure on  $\mathcal{X}$ . Therefore,  $\Phi_p^+(\mathbf{M}_\alpha) \geq \Phi_p^+(\mathbf{M}'_\alpha)$ , where  $\mathbf{M}_\alpha = \mathbf{M}[(1 - \alpha)\xi_0 + \alpha\tilde{\mu}] = (1 - \alpha) \mathbf{M}_0 + \alpha \int_{\mathcal{X}} \mathbf{x} \mathbf{x}^\top \tilde{\mu}(d\mathbf{x})$  and  $\mathbf{M}'_\alpha = (1 - \alpha) \mathbf{M}_0 + (\alpha/\rho) \sum_{i=1}^s \mathbf{v}_i \mathbf{v}_i^\top$ , with  $\rho = \sum_{i=1}^s \gamma_i^2$ . The eigenvector decomposition of  $\mathbf{M}'_\alpha$  gives

$$\Phi_p^+(\mathbf{M}'_\alpha) = \left\{ \frac{1}{m} \left[ (1 - \alpha)^{-p} \left( \sum_{i=s+1}^m \lambda_i^{-p} \right) + \alpha^{-p} \frac{s}{\rho^{-p}} \right] \right\}^{-1/p}$$

which reaches its maximum value for  $\alpha = \alpha^* = [1 + (\rho^{-p} \sum_{i=s+1}^m \lambda_i^{-p}/s)^{1/(p+1)}]^{-1} \in (0, 1)$ . It implies that  $\Phi_p^+(\mathbf{M}_{\alpha^*}) \geq \Phi_p^+(\mathbf{M}'_{\alpha^*}) > \Phi_p^+(\mathbf{M}_0)$ ; that is,  $\phi_p[(1 - \alpha^*)\xi_0 + \alpha^*\tilde{\mu}] > \phi_p(\xi_0)$  and  $\xi_0$  is not optimal.  $\blacksquare$

*Proof of Th 2.* The proof is in three parts. In (i) we show that for given  $\alpha$  and  $\gamma_*$  the equations (13), (14) with  $\omega_1 \leq \omega_2$  have a unique solution  $\omega_1^*(\alpha, \gamma_*)$  for  $\omega_1$ , with  $\omega_1^*(\alpha, \gamma_*) \in ((\alpha/\gamma_*)^{1/(p+1)}, (1/\gamma_*)^{1/(p+1)})$ . Then in (ii) we show that this solution is non-decreasing in  $\alpha$ , so that the required lowest bound is obtained for  $\alpha = \underline{b}_1/t$ , see (11). Finally, in (iii) we consider the case when  $t_*$  is unknown.

(i) Expressing  $\omega_2$  as a function of  $\omega_1$  using (13), we obtain  $\omega_2 = f_1(\omega_1) = (1 + \beta - \alpha\omega_1)/(1 - \alpha)$ , i.e., a decreasing linear function of  $\omega_1$  with slope  $-\alpha/(1 - \alpha)$  and such that  $f_1[(1 + \beta)/\alpha] = 0$ . Doing the same with (14), we obtain  $\omega_2 = f_2(\omega_1)$  with  $f_2(\cdot)$  decreasing and concave for  $\omega_1 \in ((\alpha/\gamma_*)^{1/(p+1)}, \infty)$ ,  $f_2(\theta)$  tending to infinity when  $\theta$  approaches  $(\alpha/\gamma_*)^{1/(p+1)}$  from above and  $\lim_{\theta \rightarrow \infty} f_2(\theta) = 1/\alpha - 1$ . Note that (15), (16) imply that  $(\alpha/\gamma_*)^{1/(p+1)} < (1/\gamma_*)^{1/(p+1)} < (1 + \beta)/\alpha$ . Therefore,  $f_2(\theta) > f_1(\theta)$  for  $\theta$  close enough to  $(\alpha/\gamma_*)^{1/(p+1)}$  or large enough.

Denote  $f'_2(\theta) = df_2(\theta)/d\theta$  and consider  $\theta_* = (1/\gamma_*)^{1/(p+1)}$ . Direct calculations indicate that  $f_2(\theta_*) = \theta_*$ ,  $f'_2(\theta_*) = -\alpha/(1 - \alpha)$  with, moreover,  $f_1(\theta_*) > f_2(\theta_*)$  when  $\beta > 0$ , i.e., when  $\epsilon > 0$ , due to (15) and (16). Two solutions  $\omega_{1,a}^*, \omega_{1,b}^*$  thus exist for (13), (14), with  $\omega_{1,a}^* < \theta_* < \omega_{1,b}^*$ . Only

$\omega_{1,a}^*$  is such that the associated  $\omega_{2,a}^*$  satisfies  $\omega_{2,a}^* > \omega_{1,a}^*$ . When  $\epsilon = 0$ , then  $f_1(\theta_*) = f_2(\theta_*) = \theta_*$  and the two solutions  $\omega_{1,a}^*, \omega_{1,b}^*$  are confounded and equal  $\theta_*$  (and also coincide with  $\omega_{2,a}^*$  and  $\omega_{2,b}^*$ ). The equations (13) and (14) with  $\omega_1 \leq \omega_2$  thus always have a unique solution  $\omega_1^*(\alpha, \gamma_*)$  and this solution belongs to the interval  $((\alpha/\gamma_*)^{1/(p+1)}, \theta_*]$ .

(ii) Applying the implicit function theorem to (13), (14) we obtain that the solution  $\omega_1^*(\alpha, \gamma_*)$  satisfies

$$\begin{aligned} \frac{\partial \omega_1^*(\alpha, \gamma_*)}{\partial \alpha} &= \frac{(p+1)(\omega_1^*)^{p+2}(\omega_1^* - \omega_2^*) + \omega_1^* \omega_2^* [(\omega_2^*)^{p+1} - (\omega_1^*)^{p+1}]}{\alpha(p+1)[(\omega_2^*)^{p+2} - (\omega_1^*)^{p+2}]} \\ &= \frac{\omega_1^*}{\alpha(p+1)(z^{p+2} - 1)} [(p+1)(1-z) + z(z^{p+1} - 1)], \end{aligned}$$

where  $z = \omega_2^*/\omega_1^* \geq 1$ . Denote  $f(z) = (p+1)(1-z) + z(z^{p+1} - 1)$ , its derivative is  $df(z)/dz = (p+2)(z^{p+1} - 1)$  so that  $f(z) \geq f(1) = 0$ . Since (11) gives  $\alpha \geq \underline{b}_1/t$ , one has  $\omega_1^*(\alpha, \gamma_*) \geq \omega_1^*(\underline{b}_1/t, \gamma_*)$ . The substitution of  $[\omega_1^*(\underline{b}_1/t, \gamma_*)]^{p+1}$  for  $\underline{\lambda}_1$  in (7) concludes the proof for the case when  $t_*$  is known.

(iii) When  $t_*$  is unknown, an upper bound can be substituted for  $t_*$  in (12). Using (15), (16), this amounts at replacing  $\gamma_*$  by the upper bound  $\gamma = \max\{1, (1 + \epsilon/t)^{-p}\}$ . The necessary conditions (9), (10) with  $\underline{\lambda}_1 = [\omega_1^*(\underline{b}_1/t, \gamma)]^{p+1}$  then give (17).

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