Removing inessential points in c-and A-optimal design

Luc Pronzato, Guillaume Sagnol

Removing inessential points in c-and A-optimal design

Luc Pronzato* and Guillaume Sagnol†

June 15, 2020

Abstract

A design point is inessential when it does not contribute to an optimal design, and can therefore be safely discarded from the design space. We derive three inequalities for the detection of such inessential points in c-optimal design: the first two are direct consequences of the equivalence theorem for c-optimality; the third one is derived from a second-order cone programming formulation of c-optimal design. Elimination rules for A-optimal design are obtained as a byproduct. When implemented within an optimization algorithm, each inequality gives a screening test that may provide a substantial acceleration by reducing the size of the problem online. Several examples are presented with a multiplicative algorithm to illustrate the effectiveness of the approach.

Keywords: A-optimal design; c-optimal design; Inessential Point; Screening Test; Support Point.
AMS subject classifications: 62K05, 62J07, 90C46

1 Introduction

Let $\mathbb{H} = \{\mathbf{H}_i,\, i = 1, \ldots, q\}$ denote a set of $m \times m$ symmetric non-negative definite matrices and denote by $\mathscr{H}$ its convex hull. We assume that the linear span of $\mathbb{H}$ contains a nonsingular matrix. A design corresponds to a probability measure on $\mathbb{H}$, that is, to vector of weights $\mathbf{w} = (w_1, \ldots, w_q)^\top$ in the probability simplex $\mathscr{P}_q = \{\mathbf{w} \in \mathbb{R}^q,\, w_i \geq 0 \text{ for all } i \text{ and } \sum_{i=1}^q w_i = 1\}$. The extension to designs ξ defined as probability measures on an arbitrary compact set of matrices $\mathbf{H}_t$ is straightforward, but for the sake of simplicity in the rest of the paper we shall restrict the presentation to the discrete case. A c-optimal design, associated with a nonzero vector $\mathbf{c} \in \mathbb{R}^m$, is defined by a vector $\mathbf{w}^*$ that minimizes

$$\phi(\mathbf{w}) = \Phi[\mathbf{M}(\mathbf{w})] = \mathbf{c}^\top \mathbf{M}^-(\mathbf{w})\mathbf{c} \tag{1.1}$$

with respect to $\mathbf{w}$, with $\mathbf{M}(\mathbf{w})$ the (information) matrix

$$\mathbf{M}(\mathbf{w}) = \sum_{i=1}^q w_i\, \mathbf{H}_i \tag{1.2}$$

and $\mathbf{M}^-$ a pseudo-inverse of $\mathbf{M}$. We set $\phi(\mathbf{w}) = \infty$ when $\mathbf{c}$ does not belong to the column space of $\mathbf{M}(\mathbf{w})$; the value of $\phi(\mathbf{w})$ does not depend on the choice of the pseudo-inverse $\mathbf{M}^-$.

*CNRS, Université Côte d'Azur, I3S, France, Luc.Pronzato@cnrs.fr (corresponding author)
†Institut für Mathematik, Technische Universität Berlin, sagnol@math.tu-berlin.de

A typical example is when $\mathbf{H}_i = \mathbf{a}_i\mathbf{a}_i^\top$ for all i, with $\mathbf{a}_i$ the vector of regressors in the model with observations

$$Y_i = \mathbf{a}_i^\top \boldsymbol{\theta} + \varepsilon_i \,, \tag{1.3}$$

parameters $\boldsymbol{\theta}$ and i.i.d. errors ε_i having zero mean and variance σ^2. Suppose that n observations are collected according to the design $\mathbf{w} \in \mathscr{P}_q$, with $\mathbf{w}$ such such that $nw_i \in \mathbb{N}$ for all i. Then, $\sigma^2\,\phi(\mathbf{w})/n$ is the variance of $\mathbf{c}^\top\widehat{\boldsymbol{\theta}}^n$, with $\widehat{\boldsymbol{\theta}}^n$ the Best Linear Unbiased Estimator (BLUE) of $\boldsymbol{\theta}$.

When the observations $\mathbf{Y}_i$ are multivariate, with $\mathbf{Y}_i = \mathbf{A}_i^\top\boldsymbol{\theta} + \boldsymbol{\varepsilon}_i$ in $\mathbb{R}^q$ where the errors $\boldsymbol{\varepsilon}_i$ have the $q \times q$ covariance matrix $\boldsymbol{\Sigma}_i$, $\sigma^2\,\phi(\mathbf{w})/n$ is still equal to $\mathsf{var}(\mathbf{c}^\top\widehat{\boldsymbol{\theta}}^n)$, with now

$$\mathbf{H}_i = \mathbf{A}_i\boldsymbol{\Sigma}_i^{-1}\mathbf{A}_i^\top \tag{1.4}$$

in $\mathbf{M}(\mathbf{w})$, and each $\mathbf{H}_i$ may have rank larger than 1; see for instance Harman and Trnovská (2009) for the case of D-optimal design that maximizes $\det[\mathbf{M}(\mathbf{w})]$. When setting a normal prior $\mathscr{N}(\boldsymbol{\theta}^0, \boldsymbol{\Sigma})$ on $\boldsymbol{\theta}$ in the regression model (1.3), with $\boldsymbol{\Sigma}$ having full rank, and when the errors ε_i are normal $\mathscr{N}(0, \sigma^2)$, the posterior variance of $\mathbf{c}^\top\boldsymbol{\theta}$ after n observations is $\sigma^2\,\phi(\mathbf{w})/n$, with $\phi(\mathbf{w})$ given by (1.1) and

$$\mathbf{H}_i = \mathbf{a}_i\mathbf{a}_i^\top + \sigma^2\,\boldsymbol{\Sigma}^{-1}/n = [\mathbf{a}_i \quad n^{-1/2}\sigma\boldsymbol{\Sigma}^{-1/2}]\,[\mathbf{a}_i \quad n^{-1/2}\sigma\boldsymbol{\Sigma}^{-1/2}]^\top \tag{1.5}$$

in (1.2); one may refer in particular to Pilz (1983) for a thorough exposition on optimal design for Bayesian estimation (Bayesian optimal design). When $\mathbf{H}_i$ is given by (1.5), c-optimal design is equivalent to the minimization of $\mathbf{c}'^\top\mathbf{M}^-(\mathbf{w})\mathbf{c}'$ where $\mathbf{c}' = \boldsymbol{\Sigma}^{1/2}\mathbf{c}$, $\mathbf{M}(\mathbf{w}) = \sum_{i=1}^q w_i\,\mathbf{H}_i'$, and $\mathbf{H}_i' = \boldsymbol{\Sigma}^{1/2}\mathbf{a}_i\mathbf{a}_i^\top\boldsymbol{\Sigma}^{1/2} + (\sigma^2/n)\,\mathbf{I}_m$ for all i, so that we can assume that $\boldsymbol{\Sigma} = \mathbf{I}_m$, the m-dimensional identity matrix, without any loss of generality. Other cases of interest correspond to A- and L-optimality, they will be considered in Section 4.

In general, not all $\mathbf{H}_i$ contribute to an optimal design $\mathbf{w}^*$ as some of the weights w_i^* equal zero. We shall say that such an $\mathbf{H}_i$, which does not support an optimal design, is inessential. In Section 2 we show that any design $\mathbf{w}$ yields two simple inequalities that must be satisfied by an $\mathbf{H}_i$ that contributes to an optimal design. Any $\mathbf{H}_i$ that does not satisfy these screening inequalities is therefore inessential and can be safely eliminated from $\mathbb{H}$ — we shall sometimes speak of (design-) point elimination instead of matrix elimination, which is all the more appropriate when $\mathbf{H}_i$ has the form (1.5) and the $\mathbf{a}_i$ are seen as points in $\mathbb{R}^m$. The idea originated from Pronzato (2003) and Harman and Pronzato (2007) for D-optimal design (and for the construction of the minimum-volume ellipsoid containing a set of points); it was further extended to Kiefer's φ_p criteria (Pronzato, 2013), to E-optimal design (Harman and Rosa, 2019), and to the elimination of inessential points in the smallest enclosing ball problem (Pronzato, 2019). In Section 3, we use the Second-Order Cone Programming formulation of c-optimal design of Sagnol (2011) to derive a third screening inequality. Since A-optimal design can be seen as c-optimal design in a higher dimensional space, see Sagnol (2011), the same screening inequalities can be used to eliminate inessential points in A-optimal design. This is considered in Section 4, where a comparison is made with the elimination method of Pronzato (2013). The inequalities proposed in the paper become more stringent when $\mathbf{w}$ approaches an optimal design $\mathbf{w}^*$, which can be used to accelerate the construction of an optimal design. The examples of Section 5 provide an illustration for the particular case of a "multiplicative algorithm", classical in optimal design, but elimination of inessential could benefit any other algorithm.

2 Elimination of inessential points by the equivalence theorem

2.1 Optimality conditions

The function $\mathbf{M} \to \Phi(\mathbf{M}) = \mathbf{c}^\top \mathbf{M}^- \mathbf{c}$ is convex on the set $\mathbb{M}^{\geq}$ of symmetric non-negative definite matrices. When $\mathbf{M}$ has full rank, the directional derivative of Φ at $\mathbf{M}$ in the direction $\mathbf{M}'$, defined by

$$F_\Phi(\mathbf{M}, \mathbf{M}') = \lim_{\alpha \to 0^+} \frac{\Phi[(1-\alpha)\mathbf{M} + \alpha \mathbf{M}'] - \Phi(\mathbf{M})}{\alpha},$$

equals

$$F_\Phi(\mathbf{M}, \mathbf{M}') = -\mathbf{c}^\top \mathbf{M}^{-1}(\mathbf{M}' - \mathbf{M})\mathbf{M}^{-1}\mathbf{c}.$$

Denote $\Phi_* = \Phi(\mathbf{M}_*) = \min_{\mathbf{w} \in \mathscr{P}_q} \Phi[\mathbf{M}(\mathbf{w})]$, with $\mathbf{M}_* = \mathbf{M}(\mathbf{w}^*)$ a c-optimal matrix in $\mathscr{H}$, and define

$$\delta = \delta(\mathbf{M}) = \frac{\max_{\mathbf{M}' \in \mathscr{H}} \mathbf{c}^\top \mathbf{M}^{-1}\mathbf{M}'\mathbf{M}^{-1}\mathbf{c} - \mathbf{c}^\top \mathbf{M}^{-1}\mathbf{c}}{\mathbf{c}^\top \mathbf{M}^{-1}\mathbf{c}}, \tag{2.1}$$

where the maximum is attained for $\mathbf{M}'$ equal to some $\mathbf{H}_i \in \mathbb{H}$. The convexity of Φ implies that $\Phi(\mathbf{M}') \geq \Phi(\mathbf{M}) + F_\Phi(\mathbf{M}, \mathbf{M}')$ for all $\mathbf{M}$, $\mathbf{M}'$ in $\mathscr{H}$, that is,

$$\Phi(\mathbf{M}') \quad \geq \quad 2\,\Phi(\mathbf{M}) - \mathbf{c}^\top \mathbf{M}^{-1}\mathbf{M}'\mathbf{M}^{-1}\mathbf{c} \text{ for all } \mathbf{M},\, \mathbf{M}' \in \mathscr{H}.$$

Similarly, using the stronger property that the function $\mathbf{M} \to 1/\Phi(\mathbf{M})$ is concave, we obtain

$$\Phi(\mathbf{M}') \quad \geq \quad \frac{\Phi^2(\mathbf{M})}{\mathbf{c}^\top \mathbf{M}^{-1}\mathbf{M}'\mathbf{M}^{-1}\mathbf{c}} \text{ for all } \mathbf{M},\, \mathbf{M}' \in \mathscr{H}. \tag{2.2}$$

A matrix $\mathbf{M}_*$ is c-optimal if and only if $F_\Phi(\mathbf{M}_*, \mathbf{M}) \geq 0$ for all $\mathbf{M} \in \mathscr{H}$. Therefore, when $\mathbf{M}_*$ has full rank (which is necessarily the case when $\text{rank}(\mathbf{H}) = m$ for all $\mathbf{H} \in \mathbb{H}$), $\mathbf{M}_*$ is c-optimal if and only if

$$\mathbf{c}^\top \mathbf{M}_*^{-1}\mathbf{H}\mathbf{M}_*^{-1}\mathbf{c} \leq \Phi_* \text{ for all } \mathbf{H} \in \mathbb{H}. \tag{2.3}$$

Substituting $\mathbf{H}_i$ for $\mathbf{H}$, since $\mathbf{M}_* = \sum_{i:\mathbf{w}_i^*>0} \mathbf{w}_i^* \mathbf{H}_i$ we obtain that

$$\mathbf{c}^\top \mathbf{M}_*^{-1}\mathbf{H}_i\mathbf{M}_*^{-1}\mathbf{c} = \Phi_* \text{ for all } \mathbf{H}_i \text{ such that } w_i^* > 0. \tag{2.4}$$

The properties (2.3, 2.4) correspond to what is called "equivalence theorem" in optimal design, which is central to major developments in the field since the pioneering work of Kiefer and Wolfowitz (1960) on D-optimal design; see for instance Silvey (1980); Pukelsheim (1993). The equivalence theorem takes a more complicated form when $\mathbf{M}_*$ is singular, so that Φ is not differentiable at $\mathbf{M}_*$; see Pukelsheim (1993, Chap. 2, 4). When $\mathbf{c}$ belongs to the column space of $\mathbf{M}$, the directional derivative at $\mathbf{M}$ in the direction $\mathbf{M}'$ is then

$$F_\Phi(\mathbf{M}, \mathbf{M}') = \max_{\mathbf{A}:\mathbf{M}\mathbf{A}\mathbf{M}=\mathbf{M}} -\mathbf{c}^\top \mathbf{A}^\top(\mathbf{M}' - \mathbf{M})\mathbf{A}\mathbf{c},$$

and the equivalence theorem indicates that $\mathbf{M}_*$ is c-optimal if and only if $\mathbf{c}$ belongs to the column space of $\mathbf{M}_*$ and there exists a generalized inverse $\mathbf{M}_*^-$ of $\mathbf{M}_*$ (i.e., such that $\mathbf{M}_*\mathbf{M}_*^-\mathbf{M}_* = \mathbf{M}_*$) satisfying $\mathbf{c}^\top \mathbf{M}_*^{-\top}\mathbf{H}\mathbf{M}_*^-\mathbf{c} \leq \Phi_*$ for all $\mathbf{H} \in \mathbb{H}$, with equality for all $\mathbf{H}_i$ with $w_i^* > 0$.

When all $\mathbf{H}_i$ have rank one, Elfving's theorem (1952) gives a simpler necessary and sufficient condition for c-optimality; see also (Pukelsheim, 1993, p. 50). In (Sagnol, 2011), Elfving's theorem is extended to the case of matrices $\mathbf{H}_i$ having rank larger than one; see also Section 3. The following lemma summarizes the properties that we shall use to derive screening bounds based on the equivalence theorem.

Lemma 2.1. *A c-optimal matrix* $\mathbf{M}_* = \mathbf{M}(\mathbf{w}^*)$ *satisfies*

$$\frac{1}{1+\delta}\,\Phi(\mathbf{M}) \le \Phi_* = \Phi(\mathbf{M}_*) \le \Phi(\mathbf{M}) \text{ for any full rank matrix } \mathbf{M} \in \mathscr{H} \tag{2.5}$$

and there exists a generalized inverse $\mathbf{M}_*^-$ *of* $\mathbf{M}_*$ *such that*

$$\mathbf{c}^\top \mathbf{M}_*^- \mathbf{H}_i \mathbf{M}_*^- \mathbf{c} = \Phi_* \text{ for all } \mathbf{H}_i \text{ such that } w_i^* > 0\,. \tag{2.6}$$

Proof. The first inequality in (2.5) is obtained by substituting $\mathbf{M}_*$ for $\mathbf{M}'$ in (2.2) and using (2.1) and $\max_{\mathbf{M}' \in \mathscr{H}} \mathbf{c}^\top \mathbf{M}^{-1}\mathbf{M}'\mathbf{M}^{-1}\mathbf{c} \ge \mathbf{c}^\top \mathbf{M}^{-1}\mathbf{M}_*\mathbf{M}^{-1}\mathbf{c}$; the second inequality follows from the optimality of $\mathbf{M}_*$; (2.6) is part of the equivalence theorem. □

2.2 Elimination rule

The following property allows us to eliminate inessential matrices $\mathbf{H}_i$ from $\mathbb{H}$. The proof is given in Appendix A. We denote by $\lambda_{\max}(\mathbf{A})$ and $\lambda_{\min}(\mathbf{A})$ the maximum and minimum eigenvalues, respectively, of the matrix $\mathbf{A}$.

Theorem 2.1. *Let* $\mathbf{M}$ *be any full rank matrix in* $\mathscr{H}$, $\delta = \delta(\mathbf{M})$ *be given by* (2.1), *and* $\mathbf{H}_i$ *be a matrix in* $\mathbb{H}$ *such that*

$$B_1(\mathbf{M}, \mathbf{H}_i) = \left[1 - \Delta_i \left(\frac{\delta}{1+\delta}\right)^{1/2}\right] \Phi(\mathbf{M}) - \mathbf{c}^\top \mathbf{M}^{-1}\mathbf{H}_i\mathbf{M}^{-1}\mathbf{c} > 0\,, \tag{2.7}$$

or

$$B_2(\mathbf{M}, \mathbf{H}_i) = \gamma(\kappa_i, \varphi)\,\Phi(\mathbf{M}) - \mathbf{c}^\top \mathbf{M}^{-1}\mathbf{H}_i\mathbf{M}^{-1}\mathbf{c} > 0\,, \tag{2.8}$$

where $\Delta_i = \lambda_{\max}(\mathbf{\Omega}_i) - \lambda_{\min}(\mathbf{\Omega}_i)$, $\kappa_i = \lambda_{\max}(\mathbf{\Omega}_i)/\lambda_{\min}(\mathbf{\Omega}_i)$, *with* $\mathbf{\Omega}_i = \mathbf{M}^{-1/2}\mathbf{H}_i\mathbf{M}^{-1/2}$, *and*

$$\gamma(\kappa, \varphi) = \frac{\cos^2(\omega - \varphi) + \kappa\,\sin^2(\omega - \varphi)}{\cos^2(\omega) + \kappa\,\sin^2(\omega)}\,, \quad \text{with} \quad \omega = \omega(\kappa, \varphi) = \frac{1}{2}\,\left\{\arccos\left[\frac{\kappa - 1}{\kappa + 1}\cos(\varphi)\right] + \varphi\right\}\,,$$

$\varphi = \arccos[(1+\delta)^{-1/2}]$ *and* $\mathbf{M}^{-1/2}$ *a square-root matrix of* $\mathbf{M}^{-1}$. *Then* $\mathbf{H}_i$ *does not support a c-optimal design.*

Remark 2.1. (*i*) In Theorem 2.1, (2.7) remains valid when the matrices $\mathbf{H}_i$ do not have full rank provided that $\mathbf{M}$ is nonsingular. In that case, on the one hand $\lambda_{\min}(\mathbf{\Omega}_i) = 0$ and Δ_i can be computed more efficiently as $\Delta_i = \lambda_{\max}(\mathbf{\Omega}_i) = \lambda_{\max}(\mathbf{A}_i^T\mathbf{M}^{-1}\mathbf{A}_i)$ when we write $\mathbf{H}_i = \mathbf{A}_i\mathbf{A}_i^T$. On the other hand, κ_i becomes infinite and $\gamma(\kappa_i, \varphi) = 0$ in (2.8), which therefore cannot be used to eliminate singular matrices from $\mathbb{H}$. The examples in Section 5.1 will also illustrate that $B_2(\mathbf{M}, \mathbf{H}_i)$ is more sensitive than $B_1(\mathbf{M}, \mathbf{H}_i)$ to badly conditioned matrices $\mathbf{H}_i$.

(*ii*) The precise knowledge of Δ_i is not necessary to be able to eliminate a matrix $\mathbf{H}_i$: any $\mathbf{H}_i$ such that $\mathbf{c}^\top \mathbf{M}^{-1}\mathbf{H}_i\mathbf{M}^{-1}\mathbf{c} < \left\{1 - \overline{\Delta}_i\,[\delta/(1+\delta)]^{1/2}\right\}\Phi(\mathbf{M})$ with $\overline{\Delta}_i > \Delta_i$ can be safely removed from $\mathbb{H}$. Also, for a fixed φ, $\gamma(\kappa, \varphi)$ is a decreasing function of κ, so that an overestimation of $\lambda_{\max}(\mathbf{\Omega}_i)$ and an underestimation of $\lambda_{\min}(\mathbf{\Omega}_i)$ still provide a safe elimination of $\mathbf{H}_i$ via (2.8).

(*iii*) The factor $\left\{1 - \Delta_i\,[\delta/(1+\delta)]^{1/2}\right\}$ tends to one as δ tends to zero, which renders the sieve based on (2.7) finer as $\mathbf{M}$ gets closer to an optimal matrix $\mathbf{M}_*$. Since for a given κ, $\gamma(\kappa, \varphi)$ is a decreasing function of φ, the sieve based on (2.8) becomes also finer as δ decreases.

The following result indicates that the bounds in Theorem 2.1 cannot be improved by a constant factor. The proof is given in Appendix B.

Theorem 2.2. *For any $\delta, \epsilon > 0$ and any dimension $m \geq 2$, there exists a set $\mathbb{H}$, a matrix $\mathbf{M}$ in $\mathscr{H}$ (that is, a design on $\mathbb{H}$) and a $\mathbf{H}_i \in \mathbb{H}$ supporting an optimal design such that δ equals $\delta(\mathbf{M})$ given by* (2.1) *and $B_1(\mathbf{M}, \mathbf{H}_i) + \epsilon > 0$, $B_2(\mathbf{M}, \mathbf{H}_i) + \epsilon > 0$.*

The artificial example used for the proof of Theorem 2.2 suggests that (2.8) can be more accurate than (2.7). It is not always the case, however, and Example 1 of Section 5 will present situations where (2.7) eliminates more points than (2.8).

3 Elimination of inessential points by the generalized Elfving theorem

3.1 A criterion based on Second Order Cone Programming

Write each $\mathbf{H}_i$ in $\mathbb{H}$ as $\mathbf{H}_i = \mathbf{A}_i \mathbf{A}_i^\top$ with $\mathbf{A}_i$ a $m \times \ell$ matrix; see for instance (1.4) and (1.5). Sagnol (2011) gives a generalization of Elfving theorem to multiresponse models; see also Dette and Holland-Letz (2009) for the case heteroscedastic regression models and Dette (1993) for a model-robust version of c-optimality. A consequence of this generalized Elving theorem is that c-optimal design is equivalent to a Second Order Cone Programming problem (Sagnol, 2011); Theorem 3.2 exploits this equivalence to derive a sufficient condition for elimination of an inessential $\mathbf{H}_i$.

Theorem 3.1 (Sagnol, 2011)**.** *Let $\mathbf{u}^*$ and $(\boldsymbol{\mu}^*, \mathbf{h}_1^*, \ldots, \mathbf{h}_q^*)$ be respectively primal and dual solutions of the second-order cone programs:*

$$\mathsf{P-SOCP} \quad : \quad \max_{\mathbf{u} \in \mathbb{R}^m} \mathbf{c}^\top \mathbf{u} \quad \textit{subject to } \|\mathbf{A}_i^\top \mathbf{u}\| \leq 1 \textit{ for all } i = 1, \ldots, q\,,$$

$$\mathsf{D-SOCP} \quad : \quad \min_{\boldsymbol{\mu} \in \mathbb{R}^q,\, \mathbf{h}_i, \ldots, \mathbf{h}_q \in \mathbb{R}^\ell} \sum_{i=1}^q \mu_i \quad \textit{subject to } \mathbf{c} = \sum_{i=1}^q \mathbf{A}_i \mathbf{h}_i \textit{ and } \|\mathbf{h}_i\| \leq \mu_i \textit{ for all } i = 1, \ldots, q\,.$$

Then, $\mathbf{w}^* = \boldsymbol{\mu}^* / (\sum_{i=1}^q \mu_i^*)$ defines a c-optimal design; that is, it minimizes $\phi(\mathbf{w})$ given by (1.1) *with respect to $\mathbf{w} \in \mathscr{P}_q$. Moreover, $\phi(\mathbf{w}^*) = (\sum_{i=1}^q \mu_i^*)^2 = (\mathbf{c}^\top \mathbf{u}^*)^2$ and strictly positive w_i^* correspond to indices i such that $\|\mathbf{A}_i^\top \mathbf{u}^*\| = 1$.*

Theorem 3.2. *Let $\mathbf{M} = \mathbf{M}(\mathbf{w})$ be any full-rank matrix in $\mathscr{H}$. Any matrix $\mathbf{H}_i \in \mathbb{H}$ such that*

$$B_3(\mathbf{M}, \mathbf{H}_i) = 1 + \sup_{\beta \geq \lambda_{\max}(\mathbf{A}_i^\top \mathbf{M}^{-1} \mathbf{A}_i)} \left\{ \frac{\Phi(\mathbf{M})}{(1+\delta)[\mathbf{c}^\top (\beta\, \mathbf{M} - \mathbf{H}_i)^{-1} \mathbf{c}]} - \beta \right\} > 0 \tag{3.1}$$

does not support a c-optimal design.

The proof is given in Appendix C. It relies on the construction of an upper bound t^* on $\sup_{\mathbf{z} \in \mathscr{F}(\mathbf{u})} \|\mathbf{A}_i^\top \mathbf{z}\|$, where $\mathscr{F}(\mathbf{u}) = \{\mathbf{z} \in \mathbb{R}^m : \mathbf{c}^\top \mathbf{z} \geq \mathbf{c}^\top \mathbf{u} \text{ and } \|\mathbf{A}_j^\top \mathbf{z}\| \leq 1\,,\ j = 1 \ldots, q\}$; $\mathbf{H}_i$ can be safely eliminated when $t^* < 1$. The value of t^* is obtained by solving a one-dimensional optimization problem,

$$t^* = \inf_{\beta \geq \lambda_{\max}(\mathbf{A}_i^\top \mathbf{M}^{-1} \mathbf{A}_i)} \beta - \frac{(\mathbf{c}^\top \mathbf{u})^2}{\mathbf{c}^\top (\beta\, \mathbf{M} - \mathbf{H}_i)^{-1} \mathbf{c}}\,, \tag{3.2}$$

where the function to be minimized is defined by continuity at $\beta = \lambda_{\max}(\mathbf{A}_i^\top \mathbf{M}^{-1} \mathbf{A}_i)$, see Section 3.2.

Remark 3.1. (i) Theorem 3.2 is valid whatever the rank of matrices $\mathbf{H}_i$. We have $\lambda_{\max}(\mathbf{A}_i^\top \mathbf{M}^{-1}\mathbf{A}_i) = \lambda_{\max}(\mathbf{\Omega}_i)$, where $\mathbf{\Omega}_i = \mathbf{M}^{-1/2}\mathbf{H}_i\mathbf{M}^{-1/2}$ is used in Theorem 2.1.

(ii) The determination of t^* in (C.1) need not be very precise: any upper bound smaller than one also allows us to safely eliminate $\mathbf{H}_i$. Similarly, restricting β to be larger that an upper bound on $\lambda_{\max}(\mathbf{A}_i^\top \mathbf{M}^{-1}\mathbf{A}_i)$ only makes the screening test more conservative.

The following theorem extends the result of Theorem 2.2 to the bound B_3, showing that it cannot be improved by a constant factor. The proof is in Appendix B.

Theorem 3.3. *For any $\delta, \epsilon > 0$ and any dimension $m \geq 2$, there exists a set $\mathbb{H}$, a matrix $\mathbf{M}$ in $\mathscr{H}$ (that is, a design on $\mathbb{H}$) and a $\mathbf{H}_i \in \mathbb{H}$ supporting an optimal design such that δ equals $\delta(\mathbf{M})$ given by* (2.1) *and $B_3(\mathbf{M}, \mathbf{H}_i) + \epsilon > 0$.*

3.2 Numerical calculation of $B_3(\mathbf{M}, \mathbf{H}_i)$

Consider the function $f(\cdot)$ involved in the determination of t^*, see (C.1),

$$f(\beta) = \beta - \frac{\Phi(\mathbf{M})}{(1+\delta)[\mathbf{c}^\top(\beta\,\mathbf{M} - \mathbf{H}_i)^{-1}\mathbf{c}]}\,,\ \beta > \beta_{\min} = \lambda_{\max}(\mathbf{A}_i^\top \mathbf{M}^{-1}\mathbf{A}_i)\,,$$

for which we define by continuity $f(\beta_{\min}) = \beta_{\min}$. For $\beta > \beta_{\min}$, its first and second derivatives f' and f'' are

$$f'(\beta) = 1 - \frac{\Phi(\mathbf{M})[\mathbf{u}^\top\mathbf{M}\mathbf{u}]}{(1+\delta)[\mathbf{c}^\top\mathbf{u}]^2},\ f''(\beta) = 2\,\frac{\Phi(\mathbf{M})\left\{[\mathbf{u}^T\mathbf{M}(\beta\,\mathbf{M} - \mathbf{H}_i)^{-1}\mathbf{M}\mathbf{u}][\mathbf{c}^\top\mathbf{u}] - [\mathbf{u}^\top\mathbf{M}\mathbf{u}]^2\right\}}{(1+\delta)[\mathbf{c}^\top\mathbf{u}]^3}$$

where we have denoted $\mathbf{u} = (\beta\,\mathbf{M} - \mathbf{H}_i)^{-1}\mathbf{c}$. Since $f''(\beta) > 0$ follows from Cauchy-Schwarz inequality, f is convex and can easily be minimized on $[\beta_{\min}, \infty)$. (The convexity of f is already clear by construction, as we obtained Problem (C.1) by partial minimization over a subset of variables of a convex semi-definite program, see the proof of Theorem 3.2 in Appendix C.) In the examples of Section 5 we use the simple dichotomy line search presented hereafter. The search can be stopped as soon as a β is found such that $f(\beta) < 1$ (and H_i can be eliminated), or when a lower bound $\underline{f}$ on $f(\beta)$ for $\beta \in [\beta_{\min}, \infty)$ has been determined and is such that $\underline{f} \geq 1$ (and H_i cannot be eliminated). Similarly to the definition of $f(\beta_{\min})$, we define by continuity

$$f'(\beta_{\min}) = 1 - \frac{\Phi(\mathbf{M})}{(1+\delta)\,(\mathbf{c}^\top\mathbf{M}^{-1/2}\mathbf{P}_i\overline{\mathbf{D}}_i\mathbf{P}_i^\top\mathbf{M}^{-1/2}\mathbf{c})}\,,$$

where $\mathbf{P}_i\mathbf{D}_i\mathbf{P}_i^\top$ corresponds to the eigen-decomposition of $\mathbf{\Omega}_i = \mathbf{M}^{-1/2}\mathbf{H}_i\mathbf{M}^{-1/2}$ and $\overline{\mathbf{D}}_i$ is the diagonal matrix with $\{\overline{\mathbf{D}}_i\}_{k,k} = 1$ if $\{\mathbf{D}\}_{k,k} = \beta_{\min}$ and $\{\overline{\mathbf{D}}_i\}_{k,k} = 0$ otherwise.

The fact that $\underline{f}$ in Stage 2 gives a lower bound on f is a simple consequence of its convexity. The procedure converges exponentially fast since the search interval is halved at each iteration of Stage 2: when k_1 expansions are needed at Stage 1, $k_2 = k_1 - 1 + \lceil 1/\log_2(\epsilon)\rceil$ iterations are required at Stage 2, and in general k_1 is very small (with often $k_1 = 1$). Also, the initial tests at Stage 0 and the tests $f(c) < 1$ and $\underline{f} \geq 1$ at Stage 2 frequently yield early termination.

3.3 The special case $\mathbf{H}_i = \mathbf{a}_i\mathbf{a}_i^\top$

Elimination with (2.8) cannot be used when $\mathbf{H}_i = \mathbf{a}_i\mathbf{a}_i^\top$ since $B_2(\mathbf{M}, \mathbf{H}_i) = 0$, see Remark 2.1-$(i)$. However, (2.7) and (3.1) remain valid, with $\Delta_i = \lambda_{\max}(\mathbf{A}_i^\top \mathbf{M}^{-1}\mathbf{A}_i) = \lambda_{\max}(\mathbf{\Omega}_i) = \mathbf{a}_i^\top\mathbf{M}^{-1}\mathbf{a}_i$. More importantly, the minimum t^* in (C.1) can be expressed explicitly, so that no iterative minimization is needed, and $B_1(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top) > 0$ implies $B_3(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top) > 0$; that is, B_3 is more efficient than B_1 in c-optimal design with $\mathbf{H}_i = \mathbf{a}_i\mathbf{a}_i^\top$.

Determination of t^* in (C.1) by dichotomy line search.

0) (Initial tests) Compute $\beta_{\min} = \lambda_{\max}(\mathbf{A}_i^\top \mathbf{M}^{-1} \mathbf{A}_i)$;
   if $\beta_{\min} < 1$, stop: H_i can be eliminated; otherwise, compute $f'(\beta_{\min})$;
   if $f'(\beta_{\min}) \geq 0$, stop: H_i cannot be eliminated.

1) (Determination of a search interval $[a, b]$)
   Set $a = \beta_{\min}$, $f'_a = f'_b = f'(\beta_{\min})$.
   while $f'_b < 0$, do
   | $b = 2\,a$, compute $f'_b = f'(b)$; if $f'_b < 0$, set $a = b$, $f'_a = f'_b$.

2) (Minimization of f in $[a, b]$)
   Take $0 < \epsilon \ll 1$; compute $f_a = f(a)$, $f_b = f(b)$.
   while $b - a > \epsilon\,\beta_{\min}$, do
   | set $c = (a+b)/2$ and compute $f_c = f(c)$; if $f_c < 1$, stop: H_i can be eliminated;
   | compute $f'_c = f'(c)$;
   | if $f'_c < 0$, set $a = c$, $f_a = f_c$ and $f'_a = f'_c$;
   | otherwise, set $b = c$, $f_b = f_c$ and $f'_b = f'_c$;
   | compute a lower bound on f: $\underline{f} = [f'_b\,(f_a - a\,f'_a) - f'_a\,(f_b - b\,f'_b)]/(f'_b - f'_a)$;
   | if $\underline{f} \geq 1$, stop: H_i cannot be eliminated.

Theorem 3.4. *For any full rank matrix* $\mathbf{M}$ *in* $\mathscr{H}$ *and* $\mathbf{H}_i = \mathbf{a}_i\mathbf{a}_i^\top$ *in* $\mathbb{H}$, $B_3(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top)$ *defined by* (3.1) *satisfies*

$$B_3(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top) > 0 \Longleftrightarrow \mathbf{a}_i^\top \mathbf{M}^{-1}\mathbf{a}_i \in [0,1) \cup \left(\delta_i^{(3)}, \Delta_i^{(3)}\right), \tag{3.3}$$

where

$$\delta_i^{(3)} = \frac{(1+\delta)\,(\mathbf{c}^\top\mathbf{M}^{-1}\mathbf{a}_i)^2}{\Phi(\mathbf{M})}, \quad \Delta_i^{(3)} = 1 + \frac{1}{\delta}\left[1 - (\delta_i^{(3)})^{1/2}\right]^2.$$

Moreover, if $\mathbf{H}_i$ *satisfies* (2.7), *then it also satisfies* (3.1).

Proof. Using the Sherman-Morrison-Woodbury formula for matrix inversion, we obtain that the function $f(\beta)$ in (C.1) is

$$f(\beta) = \beta - \frac{\beta\,\Phi(\mathbf{M})}{(1+\delta)\left[\Phi(\mathbf{M}) + \frac{(\mathbf{c}^\top\mathbf{M}^{-1}\mathbf{a}_i)^2}{\beta - \mathbf{a}_i^\top\mathbf{M}^{-1}\mathbf{a}_i}\right]}. \tag{3.4}$$

Direct calculation shows that $f'(\mathbf{a}_i^\top\mathbf{M}^{-1}\mathbf{a}_i) = 1 - (\mathbf{a}_i^\top\mathbf{M}^{-1}\mathbf{a}_i)/\delta_i^{(3)}$, so that $f'(\mathbf{a}_i^\top\mathbf{M}^{-1}\mathbf{a}_i) \geq 0$ is equivalent to $\Delta_i = \mathbf{a}_i^\top\mathbf{M}^{-1}\mathbf{a}_i \leq \delta_i^{(3)}$, with $\delta_i^{(3)} \leq (\delta+1)^2$ from the definition (2.1) of δ.

When $f'(\mathbf{a}_i^\top\mathbf{M}^{-1}\mathbf{a}_i) < 0$, the minimizer β^* equals $\tau\,[\tau + (\mathbf{c}^\top\mathbf{M}^{-1}\mathbf{a}_i)^2]/[\delta\,\Phi(\mathbf{M})(\mathbf{c}^\top\mathbf{M}^{-1}\mathbf{a}_i)^2]$, where $\tau = |\mathbf{c}^\top\mathbf{M}^{-1}\mathbf{a}_i|\,\delta^{1/2}\,[\Phi(\mathbf{M})(\mathbf{a}_i^\top\mathbf{M}^{-1}\mathbf{a}_i) - (\mathbf{c}^\top\mathbf{M}^{-1}\mathbf{a}_i)^2]^{1/2}$ (with $\Phi(\mathbf{M})(\mathbf{a}_i^\top\mathbf{M}^{-1}\mathbf{a}_i) \geq (\mathbf{c}^\top\mathbf{M}^{-1}\mathbf{a}_i)^2$ from Cauchy-Schwarz inequality). We then obtain that $f(\beta^*) < 1$ is equivalent to $\Delta_i < \Delta_i^{(3)}$, with $\Delta_i^{(3)} - \delta_i^{(3)} = (1 + 1/\delta)\,[(\mathbf{c}^\top\mathbf{M}^{-1}\mathbf{a}_i)/\Phi^{1/2}(\mathbf{M}) - 1]^2 \geq 0$, which completes the proof of (3.3).

Suppose that (2.7) is satisfied; that is, $B_1(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top) > 0$. It is equivalent to

$$\Delta_i < \Delta_i^{(1)} = \left(\frac{1+\delta}{\delta}\right)^{1/2}\left[1 - \frac{(\mathbf{c}^\top\mathbf{M}^{-1}\mathbf{a}_i)^2}{\Phi(\mathbf{M})}\right].$$

If $\Delta_i < 1$, then $B_3(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top) > 0$. Therefore, we only need to consider the case when $\Delta_i \geq 1$. We have

$$B_1(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top) > 0 \Longleftrightarrow (\mathbf{c}^\top\mathbf{M}^{-1}\mathbf{a}_i)^2 < T_i^{(1)} = \Phi(\mathbf{M})\left[1 - \Delta_i\left(\frac{\delta}{1+\delta}\right)^{1/2}\right].$$

Denote $T_i^{(3)} = \Phi(\mathbf{M})\,\Delta_i/(1+\delta)$. $T_i^{(3)} - T_i^{(1)}$ is an increasing function of Δ_i, and for $\Delta_i = 1$ we have $T_i^{(3)} - T_i^{(1)} = \Phi(\mathbf{M})\,\{[\delta(1+\delta)]^{1/2} - \delta\}/(1+\delta) > 0$, showing that $T_i^{(3)} - T_i^{(1)} > 0$ for all $\Delta_i \geq 1$. Therefore, $B_1(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top) > 0$ and $\Delta_i \geq 1$ imply $(\mathbf{c}^\top\mathbf{M}^{-1}\mathbf{a}_i)^2 < T_i^{(3)}$, which is equivalent to $\Delta_i > \delta_i^{(3)}$. It just remains to show that $\Delta_i^{(1)} \leq \Delta_i^{(3)}$. Direct calculation gives

$$\Delta_i^{(3)} - \Delta_i^{(1)} = \frac{1}{\delta\,(1+\delta)}\left\{(\delta_i^{(3)})^{1/2} - \frac{1}{1+[\delta/(1+\delta)]^{1/2}}\right\}^2 \geq 0\,,$$

which completes the proof. □

Figure 1 shows the regions $B_1(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top) > 0$ and $B_3(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top) > 0$ in the plane with x variable $R_i = (\mathbf{c}^\top\mathbf{M}^{-1}\mathbf{a}_i)^2/\Phi(\mathbf{M})$ and y variable Δ_i. The yellow area is a forbidden zone, due to Cauchy-Schwarz inequality $\Delta_i \geq R_i$ and the definition of δ which imposes $R_i \leq \delta + 1$. $B_1(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top) > 0$ is equivalent to Δ_i lying below the red line; it corresponds to the region colored in red. Define $\psi = (1 + 1/\delta)^{1/2} > 1$. The line $B_1 = 0$ crosses the main diagonal $\Delta_i = R_i$ at point A, with both coordinates equal to $R_i(A) = \psi/(1+\psi)$. The blue diagonal dashed-line corresponds to $\Delta_i = \delta^{(3)}(R_i)$ and the blue dashed curve to $\Delta_i = \Delta^{(3)}(R_i)$. It is tangent to the line $B_1 = 0$ at point B with coordinates $(1/[\delta\,(1+\psi)^2],\, 2\,\psi/(1+\psi))$; it is also tangent to the horizontal line $\Delta_i = 1$ at point C with coordinates $(1/(1+\delta), 1)$ and tangent to the main diagonal at point D with coordinates $(1+\delta, 1+\delta)$; C is also on the line $\Delta_i = \delta^{(3)}(R_i)$. The region $B_3(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top) > 0$ corresponds to the red region $B_3(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top) > 0$ augmented by the blue region, showing the superiority of B_3 over B_1.

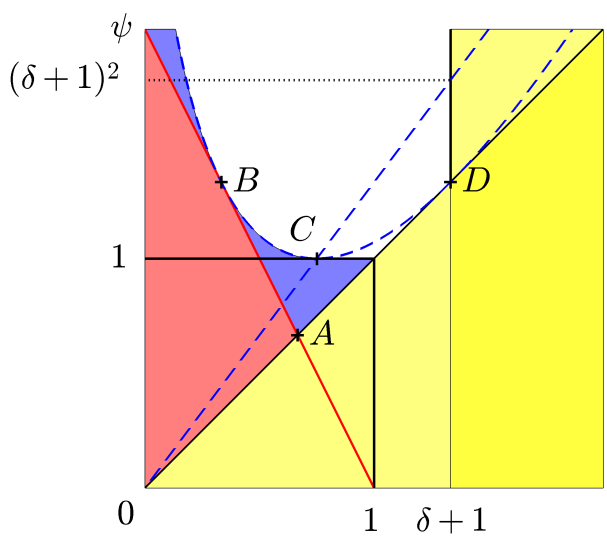

Figure 1: Regions $B_1(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top) > 0$ (red) and $B_3(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top) > 0$ (red and blue) in the plane (R_i, Δ_i), with $R_i = (\mathbf{c}^\top\mathbf{M}^{-1}\mathbf{a}_i)^2/\Phi(\mathbf{M})$; the plot is for $\delta = 1/3$.

4 Elimination of inessential points in A-optimal design

4.1 New elimination rules for A-optimal design

Denote by $\mathsf{vec}(\mathbf{A})$ the operation that stacks the columns of the $m \times n$ matrix $\mathbf{A}$ into a single $m\,n$ dimensional column vector and by $\mathbf{A} \otimes \mathbf{B}$ the Kronecker product of matrices $\mathbf{A}$ and $\mathbf{B}$. Then, for any $m \times m$ matrix $\mathbf{A}$ and $\overline{\mathbf{c}} = \mathsf{vec}(\mathbf{I}_m)$ we have $\overline{\mathbf{c}}^\top (\mathbf{I}_m \otimes \mathbf{A})\, \overline{\mathbf{c}} = \mathrm{trace}(\mathbf{A})$, and therefore, for an information matrix $\mathbf{M}(\mathbf{w})$ given by (1.2),

$$\overline{\mathbf{c}}^\top (\mathbf{I}_m \otimes \mathbf{M}^{-1}(\mathbf{w}))\, \overline{\mathbf{c}} = \mathrm{trace}[\mathbf{M}^{-1}(\mathbf{w})] = \Phi_A[\mathbf{M}(\mathbf{w})] = \phi_A(\mathbf{w})\,,$$

with ϕ_A the A-optimality criterion. Denoting $\overline{\mathbf{M}}(\mathbf{w}) = \mathbf{I}_m \otimes \mathbf{M}(\mathbf{w}) = \sum_{i=1}^q w_i\, (\mathbf{I}_m \otimes \mathbf{H}_i)$, we get

$$\phi_A(\mathbf{w}) = \overline{\mathbf{c}}^\top \overline{\mathbf{M}}^{-1}(\mathbf{w}) \overline{\mathbf{c}}\,, \tag{4.1}$$

showing that the screening bounds of Theorems 2.1 and 3.2 can also be used to eliminate inessential $\mathbf{H}_i$ in A-optimal design. We use $\overline{\mathbf{M}}^{-1}$ instead of $\overline{\mathbf{M}}^{-}$ in (4.1) since the property that $\overline{\mathbf{c}}$ belongs to the column space of the optimal matrix $\overline{\mathbf{M}}_*$ implies that the corresponding $\mathbf{M}_*$ is nonsingular, with $\phi_A(\mathbf{w}) = \infty$ for a singular $\mathbf{M}(\mathbf{w})$. We thus obtain the following result, where we use the property that, for any $m \times m$ matrix $\mathbf{A}$, $\mathbf{I}_m \otimes \mathbf{A}$ has the same eigenvalues as $\mathbf{A}$ (with multiplicities m).

Corollary 4.1. *Let $\mathbf{M}$ be any full rank matrix in $\mathscr{H}$ and $\mathbf{H}_i$ be a matrix in $\mathbb{H}$ such that*

$$B_{1,A}(\mathbf{M}, \mathbf{H}_i) = \left[1 - \Delta_i \left(\frac{\delta}{1+\delta}\right)^{1/2}\right] \Phi_A(\mathbf{M}) - \mathrm{trace}(\mathbf{M}^{-2}\mathbf{H}_i) > 0\,, \tag{4.2}$$

or

$$B_{2,A}(\mathbf{M}, \mathbf{H}_i) = \gamma(\kappa_i, \varphi)\, \Phi_A(\mathbf{M}) - \mathrm{trace}(\mathbf{M}^{-2}\mathbf{H}_i) > 0\,,$$

or

$$B_{3,A}(\mathbf{M}, \mathbf{H}_i) = 1 + \sup_{\beta \geq \lambda_{\max}(\mathbf{A}_i^\top \mathbf{M}^{-1}\mathbf{A}_i)} \left\{ \frac{\Phi_A(\mathbf{M})}{(1+\delta)\,\mathrm{trace}[(\beta\,\mathbf{M} - \mathbf{H}_i)^{-1}]} - \beta \right\} > 0\,, \tag{4.3}$$

where

$$\delta = \delta(\mathbf{M}) = \max_{i=1,\ldots,q} \frac{\mathrm{trace}(\mathbf{M}^{-2}\mathbf{H}_i)}{\Phi_A(\mathbf{M})} - 1\,, \tag{4.4}$$

and Δ_i and $\gamma(\kappa_i, \varphi)$ are defined in Theorem 2.1. Then $\mathbf{H}_i$ does not support an A-optimal design.

The case $\mathbf{H}_i = \mathbf{a}_i\mathbf{a}_i^\top$ deserves special attention here too. We cannot directly use the results of Section 3.3 since the matrix $\overline{\mathbf{H}}_i = \mathbf{I}_m \otimes \mathbf{H}_i = (\mathbf{I}_m \otimes \mathbf{a}_i)(\mathbf{I}_m \otimes \mathbf{a}_i^\top)$ is not of rank 1. However, similarly to Section 3.3, simplifications are obtained for $B_{1,A}$ and $B_{3,A}$ since $\Delta_i = \lambda_{\max}(\mathbf{A}_i^\top \mathbf{M}^{-1}\mathbf{A}_i) = \mathbf{a}_i^\top \mathbf{M}^{-1}\mathbf{a}_i$ and the test for $B_3(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top) > 0$ can be made explicit. Again, $B_{1,A}(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top) > 0$ implies $B_{3,A}(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top) > 0$, indicating that $B_{3,A}$ is more efficient than $B_{1,A}$ for A-optimal design with $\mathbf{H}_i = \mathbf{a}_i\mathbf{a}_i^\top$.

Theorem 4.1. *For any full rank matrix $\mathbf{M}$ in $\mathscr{H}$ and $\mathbf{H}_i = \mathbf{a}_i\mathbf{a}_i^\top$ in $\mathbb{H}$, $B_{3,A}(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top)$ defined by (4.3) satisfies*

$$B_{3,A}(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top) > 0 \Longleftrightarrow \mathbf{a}_i^\top \mathbf{M}^{-1}\mathbf{a}_i \in [0,1) \cup \left(\delta_i^{(3,A)}, \Delta_i^{(3,A)}\right)\,, \tag{4.5}$$

where

$$\delta_i^{(3,A)} = \frac{(1+\delta)\,\mathbf{a}_i^\top \mathbf{M}^{-2}\mathbf{a}_i}{\Phi_A(\mathbf{M})}\,,\ \Delta_i^{(3,A)} = 1 + \frac{1}{\delta}\,\left[1 - (\delta_i^{(3,A)})^{1/2}\right]^2\,.$$

Moreover, if $\mathbf{H}_i$ *satisfies* (4.2)*, then it also satisfies* (4.3)*.*

Proof. Using the Sherman-Morrison-Woodbury formula for matrix inversion, we obtain that the function $f(\beta)$ involved in the computation of $B_{3,A}$ is

$$f(\beta) = \beta - \frac{\beta\,\Phi_A(\mathbf{M})}{(1+\delta)\,\left[\Phi_A(\mathbf{M}) + \frac{\mathbf{a}_i^\top \mathbf{M}^{-2}\mathbf{a}_i}{\beta - \mathbf{a}_i^\top \mathbf{M}^{-1}\mathbf{a}_i}\right]}\,,$$

that is, an expression similar to (3.4) with $\mathbf{a}_i^\top \mathbf{M}^{-2}\mathbf{a}_i$ substituted for $(\mathbf{c}^\top \mathbf{M}^{-1}\mathbf{a}_i)^2$. The proof of (4.5) is thus similar to that of (3.3), with now $\beta^* = \tau\,[\tau + \mathbf{a}_i^\top \mathbf{M}^{-2}\mathbf{a}_i]/[\delta\,\Phi_A(\mathbf{M})\,\mathbf{a}_i^\top \mathbf{M}^{-2}\mathbf{a}_i]$ where $\tau = (\delta\,\mathbf{a}_i^\top \mathbf{M}^{-2}\mathbf{a}_i)^{1/2}\,[\Phi_A(\mathbf{M})(\mathbf{a}_i^\top \mathbf{M}^{-1}\mathbf{a}_i) - \mathbf{a}_i^\top \mathbf{M}^{-2}\mathbf{a}_i]^{1/2}$ and $\mathbf{a}_i^\top \mathbf{M}^{-2}\mathbf{a}^i \le (\mathbf{a}_i^\top \mathbf{M}^{-1}\mathbf{a}^i)\,\lambda_{\max}(\mathbf{M}^{-1}) < (\mathbf{a}_i^\top \mathbf{M}^{-1}\mathbf{a}_i)\,\Phi_A(\mathbf{M})$. The condition $B_1(\mathbf{M}, \mathbf{a}_i\mathbf{a}_i^\top) > 0$ is equivalent to

$$\Delta_i < (1 + 1/\delta)^{1/2}\,\left[1 - (\mathbf{a}_i^\top \mathbf{M}^{-2}\mathbf{a}_i)/\Phi_A(\mathbf{M})\right]\,.$$

The rest of the proof is identical to that of Theorem 3.4, with $\mathbf{a}_i^\top \mathbf{M}^{-2}\mathbf{a}_i$ substituted for $(\mathbf{c}^\top \mathbf{M}^{-1}\mathbf{a}_i)^2$. □

Remark 4.1. More generally, following the same line as in Sagnol (2011, Section 4.1), similar results can be derived for L- (linear) optimality — sometimes also called $A_{\mathbf{K}}$-optimality by some authors — where the criterion to be minimized is $\Phi_L[\mathbf{M}(\mathbf{w})] = \mathrm{trace}[\mathbf{C}\,\mathbf{M}^-(\mathbf{w})]$, with $\mathbf{C}$ symmetric nonnegative definite. Indeed, for $\mathbf{C} = \mathbf{K}\mathbf{K}^\top$, with $\mathbf{K}$ an $m \times r$ matrix, $r \le m$, we can write $\mathrm{trace}(\mathbf{C}\,\mathbf{M}^-) = \mathrm{trace}(\mathbf{K}^\top \mathbf{M}^- \mathbf{K}) = \overline{\mathbf{c}}^\top \overline{\mathbf{M}}^- \overline{\mathbf{c}}$, with $\overline{\mathbf{c}} = \mathsf{vec}(\mathbf{K})$ and $\overline{\mathbf{M}} = \mathbf{I}_r \otimes \mathbf{M}$, so that L-optimal design corresponds to a particular case of c-optimal design in a higher dimensional space. In particular, when $\mathbf{H}_i = \mathbf{a}_i\mathbf{a}_i^\top$, the function $f(\beta)$ in the computation of B_3 is

$$f(\beta) = \beta - \frac{\beta\,\Phi_L(\mathbf{M})}{(1+\delta)\,\left[\Phi_L(\mathbf{M}) + \frac{\mathbf{a}_i^\top \mathbf{M}^{-1}\mathbf{C}\mathbf{M}^{-1}\mathbf{a}_i}{\beta - \mathbf{a}_i^\top \mathbf{M}^{-1}\mathbf{a}_i}\right]}\,,$$

and the result of Theorem 4.1 remains valid when $\Phi_A(\mathbf{M})$ is replaced by $\Phi_L(\mathbf{M})$ and $\mathbf{a}_i^\top \mathbf{M}^{-2}\mathbf{a}_i$ by $\mathbf{a}_i^\top \mathbf{M}^{-1}\mathbf{C}\mathbf{M}^{-1}\mathbf{a}_i$ in $\delta^{(3,A)}$.

4.2 Comparison between screening bounds

In (Pronzato, 2013) a screening rule is proposed for all criteria of the form $\Phi_p(\mathbf{M}) = \mathrm{trace}(\mathbf{M}^{-p})$, for $p \in (-1, \infty)$. The specialization of this result to A-optimal design, which corresponds to $p = 1$, writes as follows.

Theorem 4.2 (Pronzato, 2013)**.** *Let* $\mathbf{M}$ *be any full rank matrix in* $\mathscr{H}$ *and* $\mathbf{H}_i$ *be a matrix in* $\mathbb{H}$ *such that*

$$B_{4,A}(\mathbf{M}, \mathbf{H}_i) = \omega^2\,\frac{\Phi_A(\mathbf{M})}{1+\delta} - \mathrm{trace}(\mathbf{M}^{-2}\mathbf{H}_i) > 0\,,$$

where ω *is the unique root in the interval* $(\alpha^{1/2}, 1)$ *of the fourth degree polynomial* $P(x) = (\alpha - x^2)\,(1 + \delta - \alpha\,x)^2 + (1-\alpha)^3\,x^2$*, with* δ *given by* (4.4) *and* $\alpha = \lambda_{\min}(\mathbf{M}^{-1})/\Phi_A(\mathbf{M}) < 1$*. Then* $\mathbf{H}_i$ *does not support an* A*-optimal design.*

Besides the resolution of a fourth-order polynomial equation, the calculation of $B_{4,A}(\mathbf{M},\mathbf{H}_i)$ requires the computation of the minimum eigenvalue of $\mathbf{M}^{-1}$ (or equivalently of the maximum eigenvalue of $\mathbf{M}$).

The comparison of $B_{4,A}$ with $B_{1,A}$ and $B_{3,A}$ is complicated due to the absence of an explicit expression for ω and its dependence on $\lambda_{\min}(\mathbf{M}^{-1})$.

Consider the particular situation where $\mathbf{M} = \alpha\,\mathbf{M}_*$ for some $\alpha \in (0,1)$, with $\mathbf{M}_*$ the A-optimal matrix in $\mathscr{H}$. Denote $\gamma_i = \mathrm{trace}(\mathbf{M}_*^{-2}\mathbf{H}_i)/\phi_A^*$, where $\phi_A^* = \Phi_A(\mathbf{M}_*)$ and $\gamma_i \in (0,1]$ for all i from the optimality of $\mathbf{M}_*$. Direct calculation gives $\mathrm{trace}(\mathbf{M}^{-2}\mathbf{H}_i) = (\gamma_i/\alpha^2)\,\phi_A^*$, $\delta = 1/\alpha - 1$ and $\mathrm{trace}(\mathbf{M}^{-1}\mathbf{H}_i) = \mathrm{trace}(\mathbf{M}_*^{-1}\mathbf{H}_i)/\alpha > \mathrm{trace}(\mathbf{M}^{-2}\mathbf{H}_i)/\Phi_A(\mathbf{M}) = \gamma_i/\alpha$, with $\alpha = \phi_A^*/\Phi_A(\mathbf{M})$ the A-efficiency of $\mathbf{M}$.

For $\mathbf{H}_i = \mathbf{a}_i\mathbf{a}_i^\top$, denote $t_i^* = \mathrm{trace}(\mathbf{M}_*^{-1}\mathbf{H}_i) = \mathbf{a}_i^\top\mathbf{M}_*^{-1}\mathbf{a}_i$. The definition (4.2) of $B_{1,A}$ gives

$$B_{1,A}(\mathbf{M},\mathbf{a}_i\mathbf{a}_i^\top) = \left[1 - t_i^*\,\frac{(1-\alpha)^{1/2}}{\alpha} - \frac{\gamma_i}{\alpha}\right]\Phi_A(\mathbf{M}) < \left\{1 - \frac{\gamma_i}{\alpha}\,[1+(1-\alpha)^{1/2}]\right\}\Phi_A(\mathbf{M})\,.$$

Therefore, $B_{1,A}(\mathbf{M},\mathbf{a}_i\mathbf{a}_i^\top) > 0$ is equivalent to $t_i^* < t_1(\alpha,\gamma_i) = (1-\gamma_i/\alpha)\alpha/(1-\alpha)^{1/2}$ and implies $\gamma_i < \gamma_1(\alpha) = \alpha\,[1+(1-\alpha)^{1/2}]^{-1}$. From $\omega < 1$ we obtain that $B_{4,A}(\mathbf{M},\mathbf{a}_i\mathbf{a}_i^\top) > 0$ implies $\gamma_i < \alpha^2$. If we compare with the necessary condition $\gamma_i < \gamma_1(\alpha)$ for $B_{1,A}(\mathbf{M},\mathbf{a}_i\mathbf{a}_i^\top) > 0$, we see that elimination with $B_{4,A}$ is more demanding than with $B_{1,A}$ for small α, but less demanding for $\alpha > \varphi$, the Golden-Section number $(\sqrt{5}-1)/2 \simeq 0.6180$, that is, when $\mathbf{M}$ is close to being optimal.

To make the comparison more precise, we specialize the example to the case $\mathbf{M}_* = \mathbf{I}_m$, with therefore $\mathbf{a}_i^\top\mathbf{M}_*^{-2}\mathbf{a}_i = \|\mathbf{a}_i\|^2 \le \phi_A^* = m$ and $\mathbf{M} = \alpha\mathbf{I}_m$, $\alpha \in (0,1)$. It may correspond for instance to A-optimal design in the hypercube $[-1,1]^m$ but also covers other situations. We obtain that $B_{1,A}(\mathbf{M},\mathbf{a}_i\mathbf{a}_i^\top) > 0$ is equivalent to $\|\mathbf{a}_i\|^2 < C_1(\alpha,m) = m\,\alpha/[1+m\,(1-\alpha)^{1/2}]$, and $B_{3,A}(\mathbf{M},\mathbf{a}_i\mathbf{a}_i^\top) > 0$ is equivalent to $\|\mathbf{a}_i\|^2 < \alpha$ for $\alpha \in (0,1/m]$, and to $\|\mathbf{a}_i\|^2 < C_3(\alpha,m) = m/\{1+[(m-1)(1/\alpha-1)]^{1/2}\}^2$ for $\alpha \in (1/m,1)$ (and $C_3(\alpha,m) \ge \alpha$, with $C_3(1/m,m) = 1/m$). Moreover, $B_{4,A}(\mathbf{M},\mathbf{a}_i\mathbf{a}_i^\top) = m\,\omega^2 - \|\mathbf{a}_i\|^2/\alpha$, with $\omega = \omega(m,\alpha)$ defined in Theorem 4.2, and $B_{4,A}(\mathbf{M},\mathbf{a}_i\mathbf{a}_i^\top) > 0$ is equivalent to $\|\mathbf{a}_i\|^2 < C_4(\alpha,m) = m\,\alpha^2\,\omega^2(m,\alpha)$.

The left panel of Fig. 2 shows the bounds $C_1(\alpha,m)$, $C_3(\alpha,m)$ and $C_4(\alpha,m)$ as functions of α for $m = 3$. $C_1(\alpha,m) < C_3(\alpha,m)$ for $\alpha \in (0,1)$ and any $m \ge 2$ since $B_{3,A}$ is always more efficient than $B_{1,A}$, see Theorem 4.1. On the one hand, $C_4(\alpha,m) < C_1(\alpha,m)$ on the left (and major) part of the interval $[0,1]$, which makes $B_{4,A}$ the less powerful for those α. On the other hand, for any $m \ge 2$ there exist $\alpha_1^*(m) < \alpha_3^*(m)$ in $(0,1)$ such that $C_4(\alpha,m) > C_1(\alpha,m)$ for $\alpha > \alpha_1^*(m)$ and $C_4(\alpha,m) > C_3(\alpha,m)$ for $\alpha > \alpha_3^*(m)$, which makes $B_{4,A}$ the most powerful close to optimality. The right panel of Fig. 2 shows the A-efficiency levels $\alpha_1^*(m)$ and $\alpha_3^*(m)$ above which $B_{4,A}$ is more powerful than $B_{1,A}$ and $B_{3,A}$, respectively, for $m = 2$ to 25. The numerical comparison in Section 5.3 indicates, however, that this behavior is not generic, $B_{4,A}$ being there much less powerful than $B_{1,A}$ and $B_{3,A}$.

5 Examples

We use rank-one matrices $\mathbf{H}_i = \mathbf{a}_i\mathbf{a}_i^\top$ in Section 5.3 on A-optimal design, but full rank matrices $\mathbf{H}_i = \mathbf{a}_i\mathbf{a}_i^\top + \lambda\,\mathbf{I}_m$, $\lambda > 0$, in the examples of Sections 5.1 and 5.2 which concern c-optimal design. When $\mathbf{H}_i = \mathbf{a}_i\mathbf{a}_i^\top$ for all i, c-optimal design corresponds to a linear programming problem (Harman and Jurík, 2008), and elimination of inessential $\mathbf{H}_i$ is less a problem than in the more difficult situation where $\mathrm{rank}(\mathbf{H}_i) > 1$.

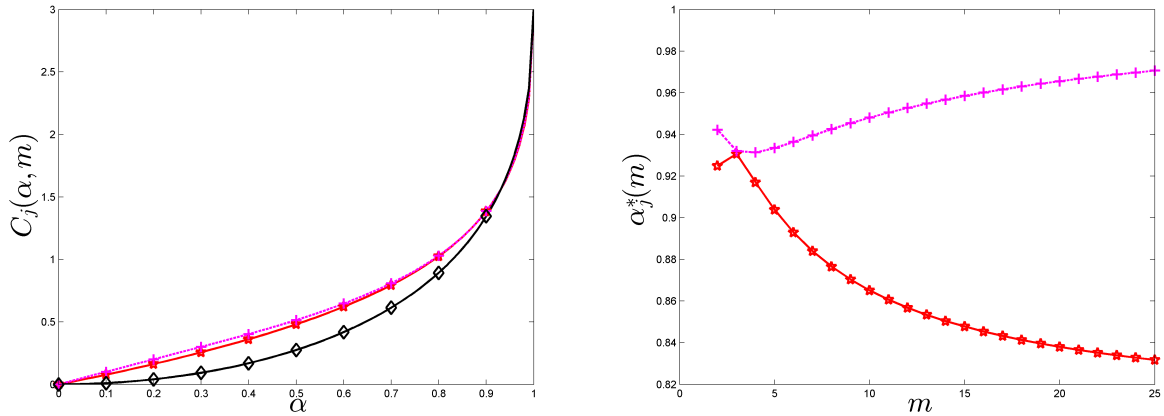

Figure 2: Left: $C_1(\alpha, m)$ (red ★), $C_3(\alpha, m)$ (magenta +) and $C_4(\alpha, m)$ (black ◊), such that $\mathbf{H}_i$ is eliminated by $B_{j,A}$ when $\|\mathbf{a}_i\|^2 < C_j$, as functions of the A-efficiency $\alpha \in (0, 1)$ for $m = 3$. Right: A-efficiencies $\alpha_1^*(m)$ (red ★) and $\alpha_3^*(m)$ (magenta +) above which $B_{4,A}$ is more powerful than $B_{1,A}$ and $B_{3,A}$ for $m = 2, \ldots, 25$.

To illustrate the potential interest of the elimination of inessential $\mathbf{H}_i$ in the construction of an optimal design, we consider the multiplicative algorithm of Fellman (1974), defined by

$$w_i^{k+1} = \frac{w_i^k \, \left[\mathbf{c}^\top \mathbf{M}^{-1}(\mathbf{w}) \mathbf{H}_i \mathbf{M}^{-1}(\mathbf{w}) \mathbf{c}\right]^{1/2}}{\sum_{j=1}^q w_i^k \, \left[\mathbf{c}^\top \mathbf{M}^{-1}(\mathbf{w}) \mathbf{H}_j \mathbf{M}^{-1}(\mathbf{w}) \mathbf{c}\right]^{1/2}} \tag{5.1}$$

for c-optimality, and

$$w_i^{k+1} = \frac{w_i^k \, \mathrm{trace}^{1/2} \left[\mathbf{M}^{-2}(\mathbf{w}) \mathbf{H}_i\right]}{\sum_{j=1}^q w_i^k \, \mathrm{trace}^{1/2} \left[\mathbf{M}^{-2}(\mathbf{w}) \mathbf{H}_j\right]} \tag{5.2}$$

for A-optimality; see also Yu (2010).

5.1 Example 1: quadratic regression

In this example $\mathbf{H}_i = \mathbf{a}_i \mathbf{a}_i^\top + \lambda \, \mathbf{I}_2$ with $\mathbf{a}_i = \mathbf{a}(t_i) = (t_i, \; t_i^2)^\top$ $(m = 2)$ and $t_i \in [0, 1]$ for all i. We take $\mathbf{c} = (1, \; c)^\top$. When $\lambda = 0$, the c-optimal design over the compact set of matrices $\mathbf{H}_t$ with $t \in [0, 1]$ is the probability measure

$$\xi_0^* = \begin{cases} \alpha^* \, \delta_{\sqrt{2}-1} + (1 - \alpha^*) \, \delta_1 & \text{if } c \in [0, \; \sqrt{2} - 1] \cup [1, \infty), \\ \delta_c & \text{otherwise,} \end{cases}$$

where $\alpha_0^* = (\sqrt{2}/2) \, (1 - c)/[2(\sqrt{2} - 1) - c]$ and δ_t denotes the Dirac delta measure at t. In the rest of the example, we take $c = (\sqrt{2} - 1)/2$, which gives a 2-point optimal design with $\alpha_0^* = (\sqrt{2}/2) \, (1 - \sqrt{2}/3)/(\sqrt{2} - 1) \simeq 0.902369$.

Direct calculation based on the optimality condition (2.3) shows that for $\lambda \geq \lambda_0 = (1/2) \, (15 + 16 \sqrt{2})/(18 + 11 \sqrt{2})$, the optimal design is $\xi_\lambda^* = \delta_1$. For $\lambda_0 \geq \lambda \geq \lambda_1 = (\sqrt{2} - 1)^3/(4 \sqrt{2})$, $\xi_\lambda^* = \delta_t$, with $t = 1$ for $\lambda = \lambda_0$, $t = \sqrt{2} - 1$ for $\lambda = \lambda_1$, and t and λ related by $\lambda = t^3 \, (\sqrt{2} + 1) \, (2t + 1 - \sqrt{2})/[2(t + 1 + \sqrt{2})]$ in between. For $\lambda < \lambda_1$, ξ_λ^* is supported on the two points $\sqrt{2} - 1$ and 1, like

ξ_0^*, and α^* can be computed numerically, with $\alpha^* \simeq 0.980081$, $\alpha^* \simeq 0.910140$ and $\alpha^* \simeq 0.902377$ for $\lambda = 10^{-2}$, $\lambda = 10^{-3}$ and $\lambda = 10^{-6}$, respectively.

First, we test and compare the capability of the inequalities $B_j(\mathbf{M}(\mathbf{w}), \mathbf{H}_i) > 0$, for $j = 1, 2, 3$, to eliminate inessential $\mathbf{H}_i$ on a set of N random designs. These designs have a fixed support $\mathbb{H}$ of size q, corresponding to $t_1 = \sqrt{2} - 1$ and $t_i = (i-2)/(q-2)$ for $i = 2, \ldots, q$; the associated weights are $w_i = (\gamma_i + \zeta_i)/[\sum_{i=1}^q (\gamma_i + \zeta_i)]$, where $\gamma_1 = \alpha^*$, $\gamma_q = (1 - \alpha^*)$, $\gamma_i = 0$ for $i \neq 1, q$, and where the ζ_i are i.i.d. in $[0, s]$. For λ small enough, the designs are close to optimality when s is close to 0. For each design generated, characterized by a vector of weights $\mathbf{w}$, we compute how many $\mathbf{H}_i$ are eliminated by $B_j(\mathbf{M}(\mathbf{w}), \mathbf{H}_i) > 0$, $j = 1, 2, 3$.

Figure 3 present box plots, constructed from the N random design, of the proportions of inessential $\mathbf{H}_i$ detected when using each test $B_j(\mathbf{M}, \mathbf{H}_i) > 0$ separately (Tj), when using pairs of tests jointly (Tj U Tk), and when using the three tests altogether (T1 U T2 U T3). We take $q = 500$, $s = 10^{-3}$, $N = 1\,000$ and $\lambda = 10^{-3}$ (left), $\lambda = 10^{-6}$ (right); $\epsilon = 0.01$ in the dichotomy procedure to compute B_3. As anticipated in Remark 2.1-(i), T2 is rather inefficient when λ is small, a typical situation when $\lambda \mathbf{I}_m$ is just a regularization term introduced to avoid singularity of the $\mathbf{H}_i$. T1 is more powerful than T2 for the two values of λ considered, but not uniformly better for $\lambda = 10^{-3}$ since the combination of T1 and T2 eliminates more points than T1 alone. Although the $\mathbf{H}_i$ have full rank, so that Theorem 3.4 does not apply, T3 always performs best on this example and combination with another bound is not helpful.

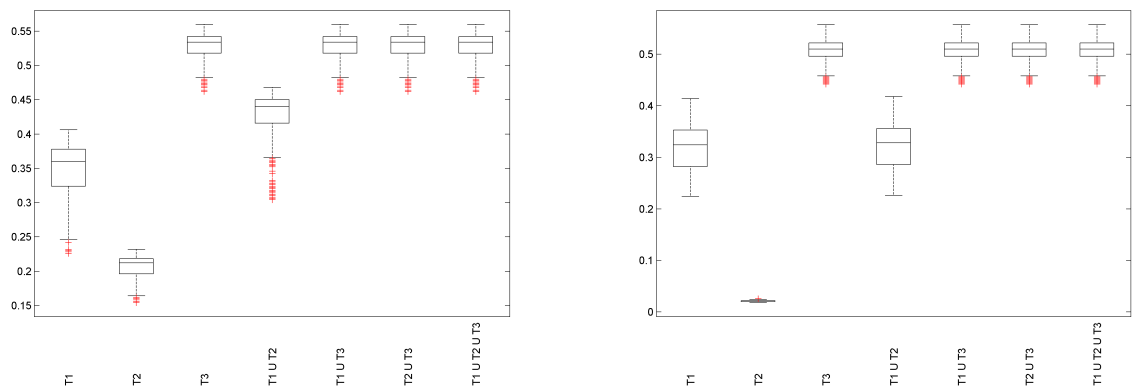

Figure 3: Box plots for 1 000 random design ($q = 500$, $s = 10^{-3}$) of proportions of inessential $\mathbf{H}_i$ when using each test separately (Tj), by pairs (Tj U Tk), and altogether (T1 U T2 U T3), for $\lambda = 10^{-3}$ (left) and $\lambda = 10^{-6}$ (right).

The left panel of Fig. 4 shows $B_1(\mathbf{M}, \mathbf{H}(t))$, $B_2(\mathbf{M}, \mathbf{H}(t))$ and $10\, B_3(\mathbf{M}, \mathbf{H}(t))$ as functions of $t \in [0, 1]$, for $\mathbf{H}(t) = \mathbf{a}(t)\mathbf{a}^\top(t) + 10^{-3}\mathbf{I}_2$ and $\mathbf{M} = \mathbf{M}(\mathbf{w}^{1\,000})$ the matrix obtained after 1 000 iterations of the multiplicative algorithm (5.1), initialized at the uniform measure on $\mathbb{H}$ that gives weight $1/q$ at each of the q matrices $\mathbf{H}_i = \mathbf{H}(t_i)$ ($q = 500$). All $\mathbf{H}_i$ such that one of the $B_j(\mathbf{M}, \mathbf{H}_i)$ is positive can be safely removed from $\mathbb{H}$. The right panel plots the proportions $\rho_j(k)$ of $\mathbf{H}_i$ such that $B_j(\mathbf{M}(\mathbf{w}^k), \mathbf{H}_i) > 0$ as a function of the iteration number k, for $k = 1, \ldots, 1\,000$.

In the rest of the example, we investigate the potential interest of eliminating inessential points in terms of computational cost (time). We take $q = 500$, $\lambda = 10^{-3}$ and $\epsilon = 0.01$ for B_3.

The left panel of Fig. 5 shows the evolution of δ given by (2.1) as a function of computational time T for the multiplicative algorithm (5.1), initialized as above, when no $\mathbf{H}_i$ is removed (black squares) and when inessential $\mathbf{H}_i$ are eliminated at iteration k if $B_j(\mathbf{M}(\mathbf{w}^k), \mathbf{H}_i) > 0$. T is measured

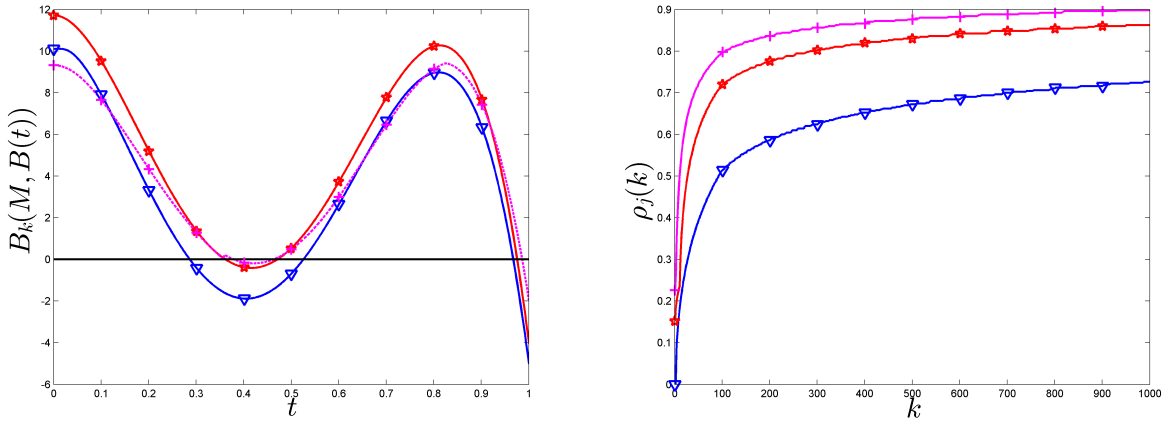

Figure 4: Left: $B_1(\mathbf{M}, \mathbf{H}(t))$ (red ★), $B_2(\mathbf{M}, \mathbf{H}(t))$ (blue ▽) and $10\, B_3(\mathbf{M}, \mathbf{H}(t))$ (magenta +) as functions of $t \in [0, 1]$, with $\mathbf{H}(t) = \mathbf{a}(t)\mathbf{a}^\top(t) + 10^{-3}\,\mathbf{I}_2$ and $\mathbf{M} = \mathbf{M}(\mathbf{w}^{1\,000})$ obtained after 1 000 iterations of algorithm (5.1); all parts above the horizontal line can be removed. Right: proportion of inessential $\mathbf{H}_i$ as a function of the iteration number k ($j = 1$: red ★, $j = 2$: blue ▽, $j = 3$: magenta +).

in seconds (calculations with Matlab, on a PC with a clock speed of 2.50 GHz and 32 Go RAM), but only the comparison between curves in meaningful. It indicates that, for the multiplicative algorithm, it is more efficient not to perform any screening test than to try to eliminate points at every iteration with one of the screening test proposed in the paper. In particular, $B_3(\mathbf{M}, \mathbf{H}_i)$ has a non negligible computational cost due to dichotomy search. If we consider that the computational cost of one iteration (5.1) is roughly proportional to the size of $\mathbf{w}$, $q\,(1 - \rho_j(i))$ at iteration i for elimination by Tj, we may rescale the iteration counter k into $\sum_{i=1}^{k}(1 - \rho_j(i))$ which counts pseudo iterations accounting for the decreasing size of $\mathbf{w}^k$. The right panel of Fig. 5 provides such a comparison of computational costs that neglects the costs of the screening tests, and only shows performance in terms of proportions of points eliminated; this is in agreement with Fig. 4-right.

To reduce the total computational cost, we now perform the screening tests more rarely, every 500 iterations only. Figure 6 presents the same information as Fig. 5 in this periodic screening situation. The left panel shows that the test based on $B_1(\mathbf{M}, \mathbf{H}_i)$ is then the most powerful on this example and provides a significant acceleration of the algorithm. The curves on the right panel are confounded up to iteration $k = 500$ when the first test is performed, compare with Fig. 5.

We have stopped the algorithm after 10 000 iterations. Figure 6 indicates that removing inessential points can accelerate the algorithm by lightening the iterations, but does not reduce the number of iterations required to reach a given accuracy, as the value of δ reached after the 10 000 iterations is approximately always the same.

5.2 Example 2: uniform points in the ball $\mathscr{B}_m(\mathbf{0}, 1)$

We take $\mathbf{H}_i = \mathbf{a}_i\mathbf{a}_i^\top + \lambda\,\mathbf{I}_m$ with the $\mathbf{a}_i$ in the m-dimensional unit ball $\mathscr{B}_m(\mathbf{0}, 1)$. When the design space is the whole ball, the delta measure at $\mathbf{a}^* = \mathbf{c}/\|\mathbf{c}\|$ is c-optimal, with $\Phi(\mathbf{M}_*) = \|\mathbf{c}\|^2/(\lambda + 1)$ and, for any $\mathbf{a}_i \in \mathscr{B}_m(\mathbf{0}, 1)$, $\mathbf{c}^\top\mathbf{M}_*^{-1}\mathbf{H}_i\mathbf{M}_*^{-1}\mathbf{c} - \Phi(\mathbf{M}_*) = [(\mathbf{c}^\top\mathbf{a}_i)^2 - \mathbf{c}^\top\mathbf{c}]/(\lambda + 1)^2 \leq 0$. We take $\mathbf{c} = (1, 0, \ldots, 0)^\top$ throughout the example.

We first visualize, for the case $m = 2$, regions of the disk where design points are eliminated

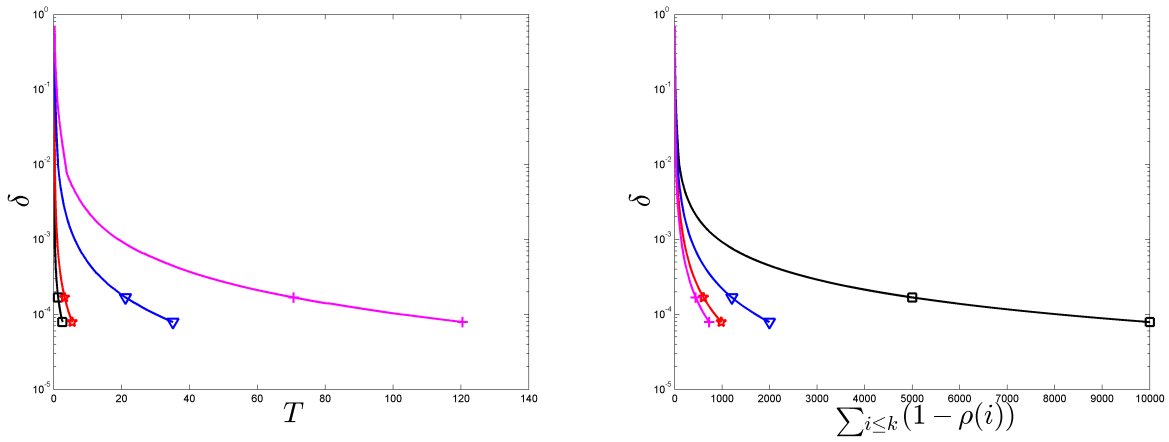

Figure 5: Left: Evolution of δ given by (2.1) as a function of computational time T for $10,000$ iterations of algorithm (5.1) with and without elimination of inessential $\mathbf{H}_i$. Right: δ as a function of pseudo iteration number. No elimination: black $\square$, elimination by T1 (red $\bigstar$), T2 (blue $\triangledown$), or T3 (magenta $+$), with screening at every iteration.

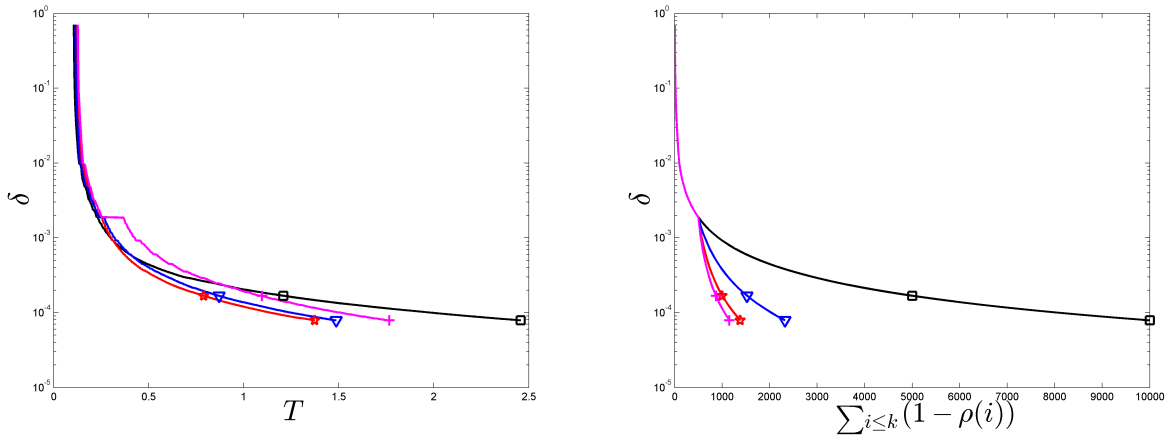

Figure 6: Same as Fig. 5 but with a screening test every 500 iterations only.

by the different screening tests. Figure 7 shows the outside contours of those regions, defined by the curves $\mathscr{A}_j = \{\mathbf{a}_i \in \mathscr{B}_2(\mathbf{0},1) : B_j(\mathbf{M}(\mathbf{w}),\mathbf{H}_i) = 0\}$, for $\lambda = 1$ (left) and $\lambda = 0.1$ (right). The matrix $\mathbf{M}(\mathbf{w})$ corresponds to a $\mathbf{w}$ close to optimality, obtained with a similar approach to previous example: we set $\mathbf{a}_1 = \mathbf{c}$ and generate $q-1$ other random $\mathbf{a}_i$ independently and uniformly distributed in $\mathscr{B}_m(\mathbf{0},1)$; the q associated weights are $w_i = (\gamma_i + \zeta_i)/[\sum_{i=1}^q(\gamma_i + \zeta_i)]$, where $\gamma_1 = 1$ and $\gamma_i = 0$ for $i > 1$, and where the ζ_i are i.i.d. in $[0, s]$. We have taken $q = 10^5$ and $s = 10^{-5}$, and the designs we use are such that $\Phi[\mathbf{M}(\mathbf{w})]/\Phi(\mathbf{M}_*) \simeq 1.14$ and 1.29 for $\lambda = 1$ and $\lambda = 0.1$, respectively. On the left panel, the regions for T2 and T3 are hardly distinguishable and the two tests dominate T1; on the right panel, T3 dominates T1 and T2, but none of them dominates the other. The complicated shapes of the contours, even in such a simple example, indicates the difficulty of determining which of the three tests is best in a given situation.

We take $\lambda = 0.1$ through the rest of the example. Figure 8 presents box plots of the proportions

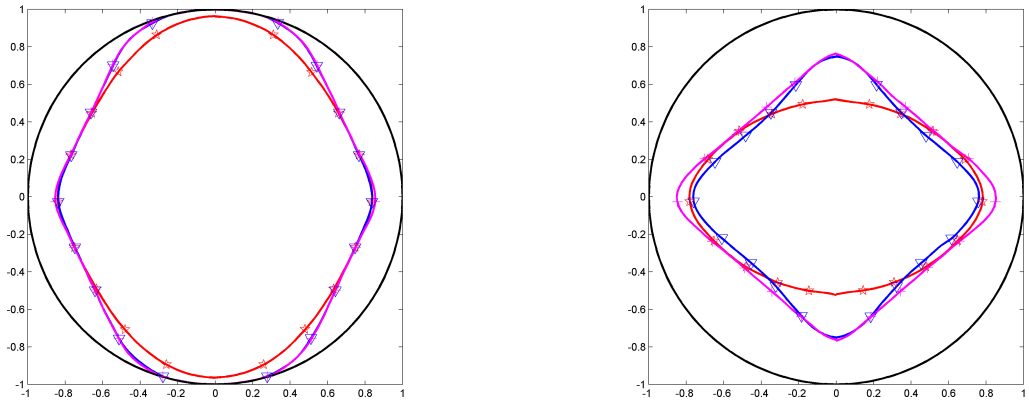

Figure 7: Outside contours of regions eliminated by the screening test T1 (red ★), T2 (blue ▽), or T3 (magenta +), for random matrices close to optimality; $\lambda = 1$ (left) and $\lambda = 0.1$ (right).

of inessential points detected when using each screening test separately (Tj), when using pairs of tests jointly (Tj U Tk), and when using the three tests altogether (T1 U T2 U T3). The plots are obtained from N random designs generated as above, with $m = 5$, $q = 1\,000$, $s = 10^{-4}$ and $N = 1\,000$. Here T1 is the less powerful, while T2 and T3 perform almost equally. There is no clear benefit in using several tests jointly.

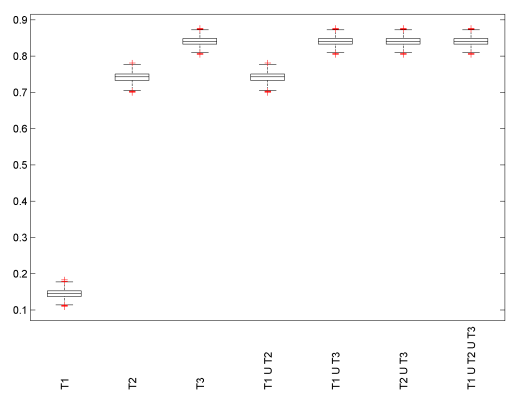

Figure 8: Box plots for 1 000 random design ($m = 5$, $\lambda = 10^{-1}$, $q = 1\,000$, $s = 10^{-4}$) of proportions of inessential $\mathbf{H}_i$ when using each test separately (Tj), by pairs (Tj U Tk), and altogether (T1 U T2 U T3).

As in Example 1, we investigate the effect of point elimination on computational time: we perform 2 000 iterations of the multiplicative algorithm, initialized at the uniform design on a set of q points independently and uniformly distributed in $\mathscr{B}_m(\mathbf{0}, 1)$, with $m = 50$ and $q = 1\,000$. Figure 9 presents the same information as Fig. 6, but when screening tests are performed more frequently, every 100 iterations. The staircase shape of the curves on the left panel is due to the long computational time required by the evaluation of $B_j(\mathbf{M}(\mathbf{w}^k), \mathbf{H}_i)$ for all $\mathbf{H}_i$ not eliminated yet:

there are 20 steps along each of the two curves, one every 100 iterations, shorter and shorter as more $\mathbf{H}_i$ are discarded. The left panel shows that T3 is hardly competitive due to its high computational cost; it becomes the most powerful if we omit this cost, see the right panel. T2 is more powerful than T1 and quicker to compute than T3; it is the most efficient in this example.

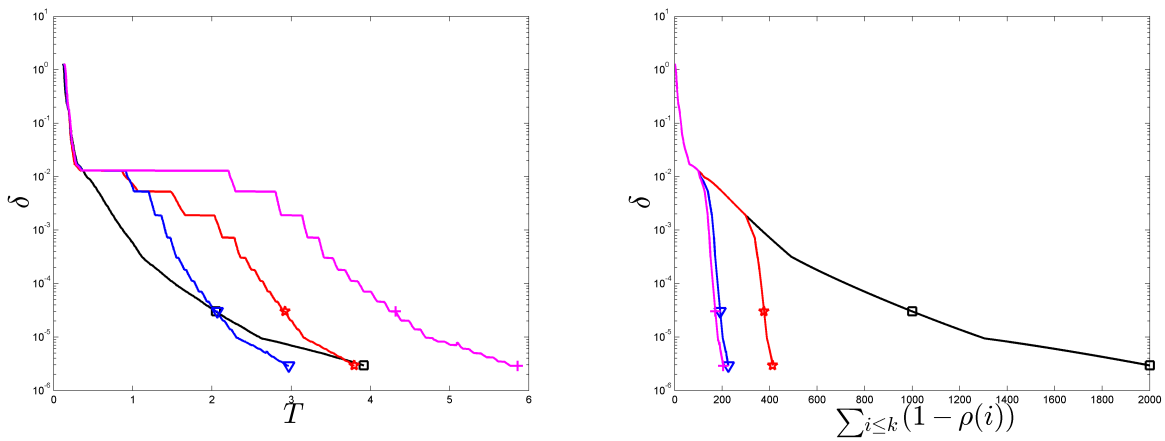

Figure 9: Left: Evolution of δ given by (2.1) as function of computational time T for algorithm (5.1) with and without elimination of inessential $\mathbf{H}_i$. Right: δ as a function of pseudo iteration number. No elimination: black $\square$, elimination by T1 (red $\bigstar$), T2 (blue $\triangledown$), or T3 (magenta $+$), with screening every 100 iterations.

5.3 Example 3: A-optimal design

We consider A-optimal design for a product-type regression model where $\mathbf{a}_i = \mathbf{a}(\mathbf{x}_i)$, $\mathbf{x}_i \in \mathscr{X} = [-1,1]^2$ and, for $\mathbf{x} = (a,b)$, $\mathbf{a}(\mathbf{x}) = (1,\, a,\, a^2,\, b,\, b^2,\, a\,b,\, a^2\,b,\, a\,b^2,\, a^2\,b^2)^\top \in \mathbb{R}^9$. The A-optimal design is the cross product of two A-optimal designs for quadratic regression on $[-1,1]$, given by $(1/4)\,\delta_{-1} + (1/2)\,\delta_0 + (1/4)\,\delta_1$, with $\mathrm{trace}(\mathbf{M}_*^{-1}) = 64$. To compute optimal designs, we discretize $\mathscr{X}$ into a regular grid with 201×201 points, which yields a set $\mathbb{H}$ of $q = 40\,401$ rank-one matrices $\mathbf{H}_i = \mathbf{a}_i\mathbf{a}_i^\top$.

The left panel of Fig. 10 shows the evolution of δ given by (2.1) as a function of computational time T for the multiplicative algorithm (5.2), initialized with the uniform distribution on $\mathbb{H}$, when no $\mathbf{H}_i$ is removed (black squares) and when inessential $\mathbf{H}_i$ are eliminated at iteration k if $B_{j,A}(\mathbf{M}(\mathbf{w}^k), \mathbf{H}_i) > 0$, for $j = 1, 3, 4$. Although the screening tests are performed at every iteration, we see that elimination of inessential points with T1 and T3 yields a significant acceleration of the algorithm. The higher computational cost of $B_{4,A}$ (it requires the computation of the minimum eigenvalue of a $m \times m$ matrix, with here $m = 9$) is not the only reason for the poorer performance of T4: the evolution of δ as a function of the pseudo iteration counter $\sum_{i=1}^k (1-\rho_j(i))$ on the right panel indicates that T4 is much less powerful than T1 and T3 on this example, a situation opposite to that in Section 4.2. The superiority of T3 over T1 is no due to a smaller computational cost (see the right panel), but to its more efficient elimination; see Theorem 4.1. When $\mathbf{H}_i = \mathbf{a}_i\mathbf{a}_i^\top$, the easy calculation of $B_{3,A}$ and its good performance in various situations make it the recommended method for support point elimination in A-optimal design.

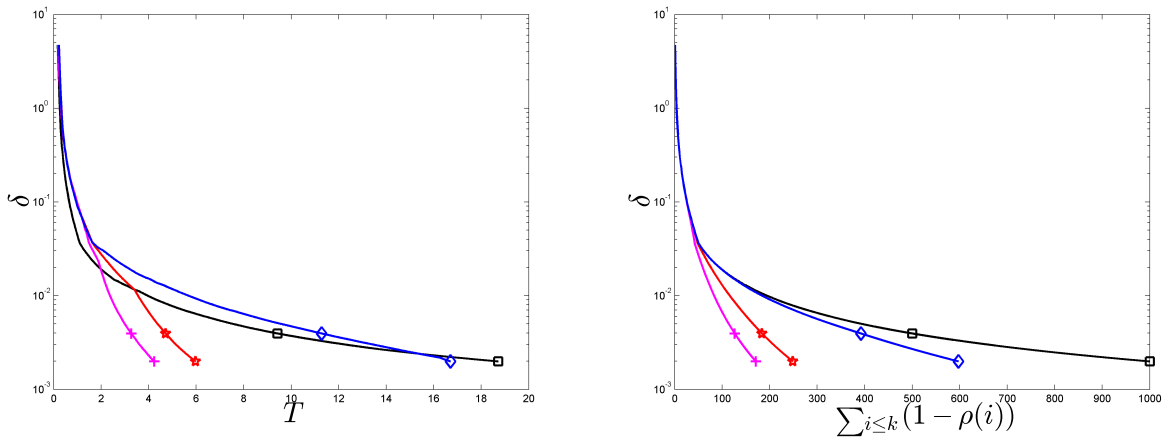

Figure 10: Left: Evolution of δ given by (2.1) as a function of computational time T for $1,000$ iterations of algorithm (5.2) with and without elimination of inessential $\mathbf{H}_i$. Right: δ as a function of pseudo iteration number. No elimination: black $\square$, elimination by T1 (red $\bigstar$), T3 (magenta $+$) or T4 (blue $\Diamond$), with screening at every iteration.

6 Conclusion and further developments

We have derived three inequalities that must be satisfied by any elementary information matrix $\mathbf{H}_i$ that contributes to a c-optimal design. The first two, B_1 and B_2, are direct consequences of the equivalence theorem for c-optimality; the third one B_3 is derived from the dual problem. Each of those inequalities can be used to safely eliminate, from a set $\mathbb{H}$ of q candidates, inessential $\mathbf{H}_i$ that cannot be support points of an optimal design. When implemented within an optimization algorithm, these inequalities can thereby provide a substantial acceleration by reducing the size of the problem online. Screening tests do not need to be done every iteration, and examples have been presented showing the value of periodic screening.

In the general situation where $\text{rank}(\mathbf{H}_i) > 1$, elimination by B_3 necessitates an iterative optimization, which induces a non-negligible computational cost and makes it less useful than B_1 and B_2. When $\text{rank}(\mathbf{H}_i) = m$, both B_1 and B_2 can be used, and the major contribution to their computational cost comes from the calculation of the maximum and minimum eigenvalues of a $m \times m$ matrix. B_2 is less efficient than B_1 when $\mathbf{H}_i$ is badly conditioned, but may perform better otherwise; since there is *a priori* no strict superiority of one bound compared to the other, we recommend to use both in parallel. When $1 < \text{rank}(\mathbf{H}_i) < m$, B_2 cannot be used and we recommend to use B_1 due to its much easier calculation than B_3. The situation is somewhat reverse when $\text{rank}(\mathbf{H}_i) = 1$: B_3 can be calculated explicitly and Theorem 3.4 shows that it is more efficient than B_1.

Since A-optimal design can be seen as a particular case of c-optimal design in a higher dimensional space, these results extend directly to A-optimal design, and the same recommendations as above can be made. In particular, when $\text{rank}(\mathbf{H}_i) = 1$, B_3 can still be calculated explicitly and Theorem 4.1 indicates that it is more efficient than B_1. Numerical examples show that in general both B_1 and B_3 outperform a screening bound already proposed for Kiefer's φ_p class of criteria, although an example has been provided indicating that the situation is reverse in particular situations.

The fact that concurrent inequalities have been derived suggests that there may still be room for improvement. The equivalence between c-optimal design and a lasso problem (Sagnol and Pauwels, 2019) is also a strong motivation for trying to derive other screening tests with low computational

cost, especially for situations with large m and q.

Appendix

A Proof of Theorem 2.1

The proof relies on the following property.

Lemma A.1. *Let $\mathbf{\Omega}$ be a $m \times m$ symmetric non-negative definite matrix with minimum and maximum eigenvalues λ_a and λ_b, respectively. Then for any pair of unit vectors $\mathbf{u}$, $\mathbf{v}$ in $\mathbb{R}^m$ making an angle $\varphi \in (-\pi/2, \pi/2)$, we have*

$$\min_{\mathbf{u},\mathbf{v}} \mathbf{u}^\top \mathbf{\Omega} \mathbf{u} - \mathbf{v}^\top \mathbf{\Omega} \mathbf{v} = -(\lambda_b - \lambda_a) \left| \sin(\varphi) \right| , \tag{A.1}$$

and

$$\min_{\mathbf{u},\mathbf{v}} \frac{\mathbf{u}^\top \mathbf{\Omega} \mathbf{u}}{\mathbf{v}^\top \mathbf{\Omega} \mathbf{v}} = \frac{\lambda_a \cos^2(\omega - \varphi) + \lambda_b \sin^2(\omega - \varphi)}{\lambda_a \cos^2(\omega) + \lambda_b \sin^2(\omega)} , \tag{A.2}$$

where

$$\omega = \frac{1}{2} \left\{ \arccos \left[\frac{\lambda_b - \lambda_a}{\lambda_b + \lambda_a} \cos(\varphi) \right] + \varphi \right\} . \tag{A.3}$$

The minimum is attained for $\mathbf{u}$ and $\mathbf{v}$ lying in the plane spanned by eigenvectors $\mathbf{e}_a$, $\mathbf{e}_b$ respectively associated with λ_a and λ_b. In that plane, there exist four configurations that yield the minimum in (A.1)*, respectively in* (A.2)*, obtained by changing the sign of one coordinate, or of both coordinates, of $\mathbf{u}$ and $\mathbf{v}$ (simultaneously) in the basis formed by $\mathbf{e}_a$ and $\mathbf{e}_b$. For* (A.1)*, one of these configurations corresponds to $\mathbf{u}$ (respectively $\mathbf{v}$) making an angle of $\pi/4 - |\varphi|/2$ (respectively, $\pi/4 + |\varphi|/2$) with $\mathbf{e}_a$. For* (A.2)*, one configuration corresponds to $\mathbf{u}$ (respectively $\mathbf{v}$) making an angle of $\omega - \varphi$ (respectively, ω) with $\mathbf{e}_a$. When $\lambda_a = 0$, $\omega = \varphi$ and $\min_{\mathbf{u},\mathbf{v}}(\mathbf{u}^\top \mathbf{\Omega} \mathbf{u})/(\mathbf{v}^\top \mathbf{\Omega} \mathbf{v}) = 0$.*

Proof. (i) Denote $f(\mathbf{u}, \mathbf{v}) = \mathbf{u}^\top \mathbf{\Omega} \mathbf{u} - \mathbf{v}^\top \mathbf{\Omega} \mathbf{v}$. We assume that $\lambda_b > \lambda_a$ to avoid the trivial solution $f(\mathbf{u}, \mathbf{v}) = 0$ for all unit vectors $\mathbf{u}$ and $\mathbf{v}$. The minimum of f cannot be achieved for $\mathbf{u}$ and $\mathbf{v}$ belonging to the null space of $\mathbf{\Omega}$, since otherwise $\mathbf{u}^\top \mathbf{\Omega} \mathbf{u} = \mathbf{v}^\top \mathbf{\Omega} \mathbf{v} = 0$. Therefore, suppose that $\mathrm{span}(\mathbf{u}, \mathbf{v})$ intersects the column space of $\mathbf{\Omega}$, and denote by $0 \leq \lambda_1 < \lambda_2$ the eigenvalues of $\Pi_{\mathbf{u},\mathbf{v}} \mathbf{\Omega} \Pi_{\mathbf{u},\mathbf{v}}$, with $\Pi_{\mathbf{u},\mathbf{v}}$ the orthogonal projector onto the plane $(\mathbf{u}, \mathbf{v})$, and by $\mathbf{e}_1$ and $\mathbf{e}_2$ the canonical orthornormal basis defined from the associated eigenvectors. In this coordinate system, we can write $\mathbf{u} = [\cos(\alpha), \sin(\alpha)]^\top$ and $\mathbf{v} = [\cos(\beta), \sin(\beta)]^\top$, which gives $f(\mathbf{u}, \mathbf{v}) = \lambda_1 [\cos^2(\alpha) - \cos^2(\beta)] + \lambda_2 [\sin^2(\alpha) - \sin^2(\beta)] = (\lambda_2 - \lambda_1) \sin(\alpha + \beta) \sin(\alpha - \beta)$ and $\mathbf{u}^\top \mathbf{v} = \cos(\alpha - \beta) = \cos(\varphi)$. The minimum of f for $\mathbf{u}, \mathbf{v}$ in this plane is thus equal to $-(\lambda_2 - \lambda_1) \left| \sin(\varphi) \right|$ and is attained when $\mathbf{u}$ and $\mathbf{v}$ are in one of the configurations indicated in the lemma. The overall minimum of f is achieved when $\mathbf{u}$ and $\mathbf{v}$ lie in the plane defined by eigenvectors $\mathbf{e}_a$ and $\mathbf{e}_b$ associated with λ_a and λ_b.

(ii) Denote now $g(\mathbf{u}, \mathbf{v}) = (\mathbf{u}^\top \mathbf{\Omega} \mathbf{u})/(\mathbf{v}^\top \mathbf{\Omega} \mathbf{v})$. When $\mathbf{\Omega}$ is singular ($\lambda_a = 0$), g reaches its minimum value zero when $\mathbf{u}$ is in the null space of $\mathbf{\Omega}$. We thus suppose that $\lambda_a > 0$ and proceed as above by writing $\mathbf{u} = [\cos(\alpha), \sin(\alpha)]^\top$ and $\mathbf{v} = [\cos(\beta), \sin(\beta)]^\top$ in the coordinate system defined by $\mathbf{e}_1$ and $\mathbf{e}_2$. Since $\mathbf{u}^\top \mathbf{v} = \cos(\alpha - \beta) = \cos(\varphi)$, we obtain

$$g(\mathbf{u}, \mathbf{v}) = \frac{\lambda_a \cos^2(\beta - \varphi) + \lambda_b \sin^2(\beta - \varphi)}{\lambda_a \cos^2(\beta) + \lambda_b \sin^2(\beta)} .$$

Direct calculation shows that the derivative with respect to β is proportional to $(\lambda_1+\lambda_2)\cos(2\beta-\varphi)-(\lambda_2-\lambda_1)\cos(\varphi)$, and the minimum g_* of $g(\mathbf{u},\mathbf{v})$ is achieved at β_* obtained by substituting λ_1 and λ_2 for λ_a and λ_b in (A.3). Finally, β_* and g_* only depend on λ_1 and λ_2 through their ratio $\kappa=\lambda_2/\lambda_1$, with g_* being a decreasing function of κ. The overall minimum of g is thus achieved when $\mathbf{u}$ and $\mathbf{v}$ lie in the plane defined by $\mathbf{e}_a$ and $\mathbf{e}_b$. □

Proof. (of Theorem 2.1) We show that any $\mathbf{H}_i$ such that $w_i^*>0$ for some c-optimal design $\mathbf{w}^*$ satisfies
(i) $\mathbf{c}^\top\mathbf{M}^{-1}\mathbf{H}_i\mathbf{M}^{-1}\mathbf{c}\geq\left\{1-\Delta_i\left[\delta/(1+\delta)\right]^{1/2}\right\}\Phi(\mathbf{M})$
and
(ii) $\mathbf{c}^\top\mathbf{M}^{-1}\mathbf{H}_i\mathbf{M}^{-1}\mathbf{c}\geq\gamma(\kappa_i,\varphi)\,\Phi(\mathbf{M})$,
where Δ_i, κ_i, φ and $\gamma(\kappa,\varphi)$ are defined in the theorem.

Let $\mathbf{M}_*=\mathbf{M}(\mathbf{w}^*)$ be a c-optimal matrix in $\mathscr{H}$, and denote by $\mathbf{M}_*^-$ its generalized inverse in the equivalence theorem, see Section 2.1. Denote $\mathbf{u}=\mathbf{M}^{-1/2}\mathbf{c}$, $\mathbf{v}=\mathbf{M}^{1/2}\mathbf{M}_*^-\mathbf{c}$, $\widehat{\mathbf{u}}=\mathbf{u}/\|\mathbf{u}\|$, $\widehat{\mathbf{v}}=\mathbf{v}/\|\mathbf{v}\|$ and $\mathbf{\Omega}_i=\mathbf{M}^{-1/2}\mathbf{H}_i\mathbf{M}^{-1/2}$ (the choice of the square root matrix unimportant). We have

$$\begin{aligned}\mathbf{u}^\top\mathbf{u} &= \Phi(\mathbf{M})\,,\\ \mathbf{u}^\top\mathbf{v} &= \Phi_*\,,\\ \mathbf{v}^\top\mathbf{v} &= \mathbf{c}^\top\mathbf{M}_*^-\mathbf{M}\mathbf{M}_*^-\mathbf{c}\leq\Phi_*\,,\end{aligned}$$

where the last equality follows from the equivalence theorem for c-optimality. Also, $\mathbf{c}^\top\mathbf{M}^{-1}\mathbf{H}_i\mathbf{M}^{-1}\mathbf{c}=\mathbf{u}^\top\mathbf{\Omega}_i\mathbf{u}$ and the equivalence theorem gives $\mathbf{c}^\top\mathbf{M}_*^-\mathbf{H}_i\mathbf{M}_*^-\mathbf{c}=\mathbf{v}^\top\mathbf{\Omega}_i\mathbf{v}=\Phi_*=\mathbf{u}^\top\mathbf{v}$. Moreover, denoting by ψ the angle between $\mathbf{u}$ and $\mathbf{v}$, we have

$$\cos(\psi)=\frac{\mathbf{u}^\top\mathbf{v}}{\|\mathbf{u}\|\,\|\mathbf{v}\|}\geq\left[\frac{\Phi_*}{\Phi(\mathbf{M})}\right]^{1/2}\geq\frac{1}{(1+\delta)^{1/2}}\,,$$

see (2.5).

We first prove (i). Using (A.1), we have

$$\begin{aligned}\mathbf{c}^\top\mathbf{M}^{-1}\mathbf{H}_i\mathbf{M}^{-1}\mathbf{c}=\mathbf{u}^\top\mathbf{\Omega}_i\mathbf{u} &= \|\mathbf{u}\|^2\,\widehat{\mathbf{u}}^\top\mathbf{\Omega}_i\widehat{\mathbf{u}}\\ &\geq \|\mathbf{u}\|^2\left(\widehat{\mathbf{v}}^\top\mathbf{\Omega}_i\widehat{\mathbf{v}}-\Delta_i\,|\sin(\psi)|\right)\\ &= \Phi(\mathbf{M})\left(\frac{\Phi_*}{\mathbf{c}^\top\mathbf{M}_*^-\mathbf{M}\mathbf{M}_*^-\mathbf{c}}-\Delta_i\,|\sin(\psi)|\right)\\ &\geq \Phi(\mathbf{M})\,(1-\Delta_i\,|\sin(\psi)|)\geq\Phi(\mathbf{M})\left\{1-\Delta_i\left[\delta/(1+\delta)\right]^{1/2}\right\}.\end{aligned}$$

This proves (i) and therefore (2.7).

We now prove (ii). Denote $R_i=(\mathbf{c}^\top\mathbf{M}^{-1}\mathbf{H}_i\mathbf{M}^{-1}\mathbf{c})/\Phi(\mathbf{M})=(\mathbf{u}^\top\mathbf{\Omega}_i\mathbf{u})/(\mathbf{u}^\top\mathbf{u})$. We can write

$$R_i=\frac{\Phi_*}{\|\mathbf{v}\|^2}\,\frac{\widehat{\mathbf{u}}^\top\mathbf{\Omega}_i\widehat{\mathbf{u}}}{\widehat{\mathbf{v}}^\top\mathbf{\Omega}_i\widehat{\mathbf{v}}}\geq\frac{\widehat{\mathbf{u}}^\top\mathbf{\Omega}_i\widehat{\mathbf{u}}}{\widehat{\mathbf{v}}^\top\mathbf{\Omega}_i\widehat{\mathbf{v}}}\,.$$

Applying (A.2) of Lemma A.1 to the right-hand side and using the property that for a fixed κ $\gamma(\kappa,\psi)$ is a decreasing function of the angle ψ, with $\gamma(\kappa,0)=1$ and $\gamma(\kappa,\pi/2)=1/\kappa$, we obtain that $R_i\geq\gamma(\kappa_i,\varphi)$ with φ such that $\cos(\varphi)=1/(1+\delta)^{1/2}$. This proves (ii) and thus (2.8). □

B Proof of Theorems 2.2 and 3.3

Proof. (of Theorem 2.2) The dimension is irrelevant, since for $m > 2$ we can consider block matrices $\mathbf{A}_m$ of the form

$$\mathbf{A}_m = \begin{pmatrix} \mathbf{A}_2 & \mathbf{O}_{2,m-2} \\ \mathbf{O}_{m-2,2} & \mathbf{I}_{m-2} \end{pmatrix},$$

with $\mathbf{A}_2$ a 2×2 matrix, $\mathbf{O}_{p,q}$ the $p \times q$ null matrix, and a vector $\mathbf{c} = (c_1, c_2, 0, \ldots, 0)^\top$. We can thus restrict our attention to the case $m = 2$. Take $\mathbb{H} = \{\mathbf{H}_1, \mathbf{H}_2, \mathbf{M}\}$ with

$$\mathbf{H}_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1+a+t \end{pmatrix}, \ \mathbf{H}_2 = \begin{pmatrix} 1+a+t & 0 \\ 0 & 1 \end{pmatrix} \text{ and } \mathbf{M} = \begin{pmatrix} 1+t & 0 \\ 0 & 1 \end{pmatrix},$$

with $a, t > 0$.

For $\mathbf{c} = (\sqrt{2}/2)\,(1,1)^\top$, the c-optimal matrix is $\mathbf{M}_* = (\mathbf{H}_1 + \mathbf{H}_2)/2$, with $\Phi_* = \Phi(\mathbf{M}_*) = 2/(2+a+t) < \Phi(\mathbf{M}) = (2+t)/[2(1+t)]$. We have

$$\mathbf{c}^\top \mathbf{M}^{-1}\mathbf{H}_1\mathbf{M}^{-1}\mathbf{c} - \mathbf{c}^\top \mathbf{M}^{-1}\mathbf{H}_2\mathbf{M}^{-1}\mathbf{c} = \frac{t(2+t)(a+t)}{2(1+t)^2}$$

which is positive for $a, t > 0$, and therefore $\delta = (\mathbf{c}^\top \mathbf{M}^{-1}\mathbf{H}_1\mathbf{M}^{-1}\mathbf{c})/\Phi(\mathbf{M}) - 1 = [t^2 + at + a/(2+t)]/(1+t)$. The matrix $\mathbf{\Omega}_2 = \mathbf{M}^{-1/2}\mathbf{H}_2\mathbf{M}^{-1/2}$ is

$$\mathbf{\Omega}_2 = \begin{pmatrix} \frac{1+a+t}{1+t} & 0 \\ 0 & 1 \end{pmatrix}.$$

Consider first the bound (2.7) and denote $b_1(a,t) = B_1(\mathbf{M}, \mathbf{H}_2) = \{1 - \Delta_2\,[\delta/(1+\delta)]^{1/2}\}\,\Phi(\mathbf{M}) - \mathbf{c}^\top \mathbf{M}^{-1}\mathbf{H}_2\mathbf{M}^{-1}\mathbf{c}$, with $\Delta_2 = \lambda_{\max}(\mathbf{\Omega}_2) - \lambda_{\min}(\mathbf{\Omega}_2) = a/(1+t)$. We obtain

$$b_1(a,t) = -\frac{a\,\{(2+t)\,[\delta/(1+\delta)]^{1/2} + 1\}}{2\,(1+t)^2}.$$

The expression of δ gives

$$a = a_\delta(t) = \frac{(2+t)(\delta + \delta t - t^2)}{(1+t)^2}, \tag{B.1}$$

which is positive for $0 < t < t_\delta = \{\delta + [\delta(4+\delta)]^{1/2}\}/2$. We then obtain $b_1(a_\delta(t), t) < 0$ for $t \in (0, t_\delta)$, with $b_1(a_\delta(t_\delta), t_\delta) = 0$ and $\mathrm{d}b_1(a_\delta(t), t)/\mathrm{d}t\big|_{t=t_\delta} > 0$ for all $\delta > 0$, with $\mathrm{d}b_1(a_\delta(t), t)/\mathrm{d}t\big|_{t=t_\delta} = 0$ for $\delta = 0$, $\mathrm{d}b_1(a_\delta(t), t)/\mathrm{d}t\big|_{t=t_\delta} = 2\,\delta^{1/2} - 3\,\delta + (3/4)\,\delta^{3/2} + \mathcal{O}(\delta^2)$ for small δ, and $\mathrm{d}b_1(a_\delta(t), t)/\mathrm{d}t\big|_{t=t_\delta}$ reaching its maximum $\simeq 0.409910$ at $\delta \simeq 0.257688$.

We proceed similarly for the bound (2.8). Denote $b_2(a,t) = B_2(\mathbf{M}, \mathbf{H}_2) = \gamma(\kappa, \varphi)\,\Phi(\mathbf{M}) - \mathbf{c}^\top \mathbf{M}^{-1}\mathbf{H}_2\mathbf{M}^{-1}\mathbf{c}$, with $\kappa = \lambda_{\max}(\mathbf{\Omega}_2)/\lambda_{\min}(\mathbf{\Omega}_2) = 1 + a/(1+t)$ and $\varphi = \arccos[(1+\delta)^{-1/2}]$. We get $b_2(a_\delta(t), t) < 0$ for $t \in (0, t_\delta)$, $b_2(a_\delta(t_\delta), t_\delta) = 0$ and $\mathrm{d}b_2(a_\delta(t), t)/\mathrm{d}t\big|_{t=t_\delta} > 0$ for all $\delta > 0$; $\mathrm{d}b_2(a_\delta(t), t)/\mathrm{d}t\big|_{t=t_\delta} = 0$ at $\delta = 0$, equals $2\,\delta^{1/2} - 11\,\delta + (99/4)\,\delta^{3/2} + \mathcal{O}(\delta^2)$ for small δ, with a maximum $\simeq 0.121304$ at $\delta \simeq 0.022087$. ($b_2(a_\delta(t), t) > b_1(a_\delta(t), t)$ for all $t \in (0, t_\delta)$, $\delta > 0$, which suggests that here (2.8) is more accurate than (2.7).)

For any $\epsilon > 0$, we can thus choose a $t_* \in (0, t_\delta)$ such that $b_2(a_\delta(t_*), t_*) + \epsilon > 0$ and $b_1(a_\delta(t_*), t_*) + \epsilon > 0$. For $t = t_*$ and $a = a_\delta(t_*)$, the inequalities $B_1(\mathbf{M}, \mathbf{H}_2) + \epsilon > 0$ and $B_2(\mathbf{M}, \mathbf{H}_2) + \epsilon > 0$ are thus satisfied although $\mathbf{H}_2$ supports the optimal design. □

Proof. (of Theorem 3.3) We use the same construction as in the proof of Theorem 2.2, and denote $b_3(a,t) = B_3(\mathbf{M},\mathbf{H}_2)$. We get $\lambda_{\max}(\mathbf{A}_2^\top \mathbf{M}^{-1}\mathbf{A}_2) = 1 + a/(1+t)$ in (C.1), the optimal β is

$$\beta^* = \frac{\delta^2\,(t+1) + \delta\,(2\,t+1) + [t/(1+t)]^{1/2}\,[\delta\,(t+1) - t^2]}{\delta\,(1+t)^2}\,.$$

It gives $b_3(a_\delta(t),t) < 0$ for $0 < t < t_\delta = \{\delta + [\delta(4+\delta)]^{1/2}\}/2$, with $a_\delta(t)$ given by (B.1), and $b_3(a_\delta(t_\delta),t_\delta) = 0$. Also, $\mathrm{d}b_3(a_\delta(t),t)/\mathrm{d}t\big|_{t=t_\delta} > 0$ for all $\delta > 0$, with $\mathrm{d}b_3(a_\delta(t),t)/\mathrm{d}t\big|_{t=t_\delta} = 0$ for $\delta = 0$, $\mathrm{d}b_3(a_\delta(t),t)/\mathrm{d}t\big|_{t=t_\delta} = 2\,\delta^{1/2} - 2\,\delta - (3/4)\,\delta^{3/2} + \mathcal{O}(\delta^2)$ for small δ, and $\mathrm{d}b_3(a_\delta(t),t)/\mathrm{d}t\big|_{t=t_\delta}$ reaching its maximum $\simeq 0.510064$ at $\delta \simeq 0.346719$. For any $\epsilon > 0$, we can thus choose a $t_* \in (0,t_\delta)$ such that $b_3(a_\delta(t_*),t_*) + \epsilon > 0$, and for $t = t_*$ and $a = a_\delta(t_*)$ we have $B_3(\mathbf{M},\mathbf{H}_2) + \epsilon > 0$ although $\mathbf{H}_2$ supports the optimal design. □

C Proof of Theorem 3.2

Proof. Define the set

$$\mathscr{F}(\mathbf{u}) = \{\mathbf{z} \in \mathbb{R}^m : \mathbf{c}^\top\mathbf{z} \geq \mathbf{c}^\top\mathbf{u} \text{ and } \|\mathbf{A}_j^\top\mathbf{z}\| \leq 1\,,\ j = 1\ldots,q\}\,,$$

where $\mathbf{u} = \mathbf{M}^{-1}\mathbf{c}/(\max_j \|\mathbf{A}_j^\top\mathbf{M}^{-1}\mathbf{c}\|)$ is feasible for $\mathsf{P-SOCP}$. Then, $\sup_{\mathbf{z}\in\mathscr{F}(\mathbf{u})} \|\mathbf{A}_i^\top\mathbf{z}\| < 1$ implies that $\|\mathbf{A}_i^\top\mathbf{u}^*\| < 1$ and, from Theorem 3.1, $\mathbf{H}_i$ cannot support an optimal design. Checking the condition $\sup_{\mathbf{z}\in\mathscr{F}(\mathbf{u})} \|\mathbf{A}_i^\top\mathbf{z}\| < 1$ requires the solution of a non-convex quadratic optimization problem, but a much simpler condition can be derived using the so-called S-procedure; see, e.g., Pólik and Terlaky (2007). Let t be an upper bound on $\sup_{\mathbf{z}\in\mathscr{F}(\mathbf{u})} \|\mathbf{A}_i^\top\mathbf{z}\|$, so that $\|\mathbf{A}_i^\top\mathbf{z}\| \leq t$ for any $\mathbf{z} \in \mathscr{F}(\mathbf{u})$. This is equivalent to

$$\begin{pmatrix} 1 \\ \mathbf{z} \end{pmatrix}^\top \begin{pmatrix} -(\mathbf{c}^\top\mathbf{u})^2 & \mathbf{0}_m^\top \\ \mathbf{0}_m & \mathbf{c}\mathbf{c}^\top \end{pmatrix} \begin{pmatrix} 1 \\ \mathbf{z} \end{pmatrix} \geq 0 \ \text{ and } \ \begin{pmatrix} 1 \\ \mathbf{z} \end{pmatrix}^\top \begin{pmatrix} 1 & \mathbf{0}_m^\top \\ \mathbf{0}_m & -\mathbf{H}_j \end{pmatrix} \begin{pmatrix} 1 \\ \mathbf{z} \end{pmatrix} \geq 0 \text{ for all } j = 1\ldots,q$$
$$\Longrightarrow \begin{pmatrix} 1 \\ \mathbf{z} \end{pmatrix}^\top \begin{pmatrix} t & \mathbf{0}_m^\top \\ \mathbf{0}_m & -\mathbf{H}_i \end{pmatrix} \begin{pmatrix} 1 \\ \mathbf{z} \end{pmatrix} \geq 0\,,$$

with $\mathbf{0}_m$ the null vector of length m. A sufficient condition for this implication is the existence of nonnegative μ and τ_j $(j = 1,\ldots,q)$ such that

$$\begin{pmatrix} t & \mathbf{0}_m^\top \\ \mathbf{0}_m & -\mathbf{H}_i \end{pmatrix} \succeq \mu \begin{pmatrix} -(\mathbf{c}^\top\mathbf{u})^2 & \mathbf{0}_m^\top \\ \mathbf{0}_m & \mathbf{c}\mathbf{c}^\top \end{pmatrix} + \sum_{j=1}^q \tau_j \begin{pmatrix} 1 & \mathbf{0}_m^\top \\ \mathbf{0}_m & -\mathbf{H}_j \end{pmatrix}\,,$$

or equivalently, $t \geq \sum_{j=1}^q \tau_j - \mu\,(\mathbf{c}^\top\mathbf{u})^2$ and $\sum_{j=1}^q \tau_j\,\mathbf{H}_j - \mathbf{H}_i \succeq \mu\,\mathbf{c}\mathbf{c}^\top$, where, for $\mathbf{A}$ and $\mathbf{B}$ two square matrices of the same size, $\mathbf{A} \succeq \mathbf{B}$ means that $\mathbf{A} - \mathbf{B}$ is nonnegative definite.

Finding the smallest $t \geq 0$ such that the above linear matrix inequality holds for some nonnegative μ and τ_j is a Semi-Definite Program (SDP), the solution of which would allow the elimination of $\mathbf{H}_i$ when $t < 1$. However, solving this SDP is probably as hard (if not harder) than solving the original problem, and we restrict the search for solutions to $\boldsymbol{\tau} = (\tau_1,\ldots,\tau_q)^\top$ being proportional to $\mathbf{w}$, that is, to $\boldsymbol{\tau} = \beta\,\mathbf{w}$ with $\beta > 0$. This shows that $\mathbf{H}_i$ can be safely eliminated if the optimal value t^* of the following simplified SDP is strictly less than 1:

$$t^* = \inf_{\beta,\mu\geq 0} \beta - \mu\,(\mathbf{c}^\top\mathbf{u})^2 \ \text{ subject to } \beta\,\mathbf{M} - \mathbf{H}_i \succeq \mu\,\mathbf{c}\mathbf{c}^\top\,.$$

Any feasible β must satisfy $\beta\,\mathbf{M} \succeq \mathbf{H}_i$, that is, $\beta \geq \lambda_{\max}(\mathbf{A}_i^T\mathbf{M}^{-1}\mathbf{A}_i)$, and a simple application of the Schur-complement lemma shows that the largest feasible μ is $\mu^* = [\mathbf{c}^\top(\beta\,\mathbf{M} - \mathbf{H}_i)^-\mathbf{c}]^{-1}$. Hence the computation of t^* reduces to solving a one-dimensional optimization problem,

$$t^* = \inf_{\beta \geq \lambda_{\max}(\mathbf{A}_i^\top \mathbf{M}^{-1}\mathbf{A}_i)} \beta - \frac{(\mathbf{c}^\top \mathbf{u})^2}{\mathbf{c}^\top(\beta\,\mathbf{M} - \mathbf{H}_i)^{-1}\mathbf{c}}\,, \tag{C.1}$$

where the function $f(\cdot)$ to be minimized is defined by continuity at $\beta_{\min} = \lambda_{\max}(\mathbf{A}_i^\top\mathbf{M}^{-1}\mathbf{A}_i)$ by $f(\beta_{\min}) = \beta_{\min}$, and $\mathbf{H}_i$ can be eliminated when $t^* < 1$. From the definition (2.1) of δ, we have $(\mathbf{c}^\top\mathbf{u})^2 = \Phi(\mathbf{M})/(1+\delta)$, so that the condition $t^* < 1$ is equivalent to $B_3(\mathbf{M}, \mathbf{H}_i) > 0$, which concludes the proof. □

Acknowledgement

The work of Luc Pronzato was partly supported by project INDEX (INcremental Design of EXperiments) ANR-18-CE91-0007 of the French National Research Agency (ANR). The work of Guillaume Sagnol was supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy – The Berlin Mathematics Research Center MATH+ (EXC-20461, project ID: 390685689).

References

Dette, H. (1993). Elfving's theorem for D-optimality. *Annals of Statistics*, 21(2):753–766.

Dette, H. and Holland-Letz, T. (2009). A geometric characterization of c-optimal designs for heteroscedastic regression. *Annals of Statistics*, 37(6B):4088–4103.

Elfving, G. (1952). Optimum allocation in linear regression. *Annals Math. Statist.*, 23:255–262.

Fellman, J. (1974). On the allocation of linear observations. *Comment. Phys. Math.*, 44:27–78.

Harman, R. and Jurík, T. (2008). Computing c-optimal experimental designs using the simplex method of linear programming. *Computational Statistics and Data Analysis*, 53:247–254.

Harman, R. and Pronzato, L. (2007). Improvements on removing non-optimal support points in D-optimum design algorithms. *Statistics & Probability Letters*, 77:90–94.

Harman, R. and Rosa, S. (2019). Removal of points that do not support an E-optimal experimental design. *Statistics & Probability Letters*, 147:83–89.

Harman, R. and Trnovská, M. (2009). Approximate D-optimal designs of experiments on the convex hull of a finite set of information matrices. *Mathematic Slovaca*, 59(5):693–704.

Kiefer, J. (1974). General equivalence theory for optimum designs (approximate theory). *Annals of Stat.*, 2(5):849–879.

Kiefer, J. and Wolfowitz, J. (1960). The equivalence of two extremum problems. *Canadian Journal of Mathematics*, 12:363–366.

Pilz, J. (1983). *Bayesian Estimation and Experimental Design in Linear Regression Models*, volume 55. Teubner-Texte zur Mathematik, Leipzig. (also Wiley, New York, 1991).

Pólik, I. and Terlaky, T. (2007). A survey of the S-Lemma. *SIAM Review*, 49(3):371–418.

Pronzato, L. (2003). Removing non-optimal support points in D-optimum design algorithms. *Statistics & Probability Letters*, 63:223–228.

Pronzato, L. (2013). A delimitation of the support of optimal designs for Kiefer's ϕ_p-class of criteria. *Statistics & Probability Letters*, 83:2721–2728.

Pronzato, L. (2019). On the elimination of inessential points in the smallest enclosing ball problem. *Optimization Methods and Software*, 34(2):225–247.

Pukelsheim, F. (1993). *Optimal Experimental Design*. Wiley, New York.

Sagnol, G. (2011). Computing optimal designs of multiresponse experiments reduces to second-order cone programming. *Journal of Statistical Planning and Inference*, 141:1684–1708.

Sagnol, G. and Pauwels, E. (2019). An unexpected connection between Bayes A-optimal design criteria and the group Lasso. *Statistical Papers*, 60(2):215–234.

Silvey, S. (1980). *Optimal Design*. Chapman & Hall, London.

Yu, Y. (2010). Monotonic convergence of a general algorithm for computing optimal designs. *Annals of Statistics*, 38(3):1593–1606.