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On the regularization of singular c -optimal designs*

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Abstract

We consider the design of c -optimal experiments for the estimation of a scalar function $h(\theta)$ of the parameters θ in a nonlinear regression model. A c -optimal design ξ^* may be singular, and we derive conditions ensuring the asymptotic normality of the Least-Squares estimator of $h(\theta)$ for a singular design over a finite space. As illustrated by an example, the singular designs for which asymptotic normality holds typically depend on the unknown true value of θ , which makes singular c -optimal designs of no practical use in nonlinear situations. Some simple alternatives are then suggested for constructing nonsingular designs that approach a c -optimal design under some conditions.

Keywords. singular design, optimum design, c -optimality, D -optimality, regular asymptotic normality, consistency, LS estimation

AMS Subject Classification. 62K05, 62E20

1 Introduction

We consider experimental design for least-squares estimation in a nonlinear regression model with scalar observations

$$Y_i = Y(x_i) = \eta(x_i, \bar{\theta}) + \varepsilon_i, \quad \text{where } \bar{\theta} \in \Theta, \quad i = 1, 2, \dots \quad (1)$$

where $\{\varepsilon_i\}$ is a (second-order) stationary sequence of independent random variables with zero mean,

$$\mathbb{E}\{\varepsilon_i\} = 0 \quad \text{and} \quad \mathbb{E}\{\varepsilon_i^2\} = \sigma^2 < \infty \quad \forall i, \quad (2)$$

*This paper is dedicated to Andrej Pázman on the occasion of his 70th birthday

Θ is a compact subset of \mathbb{R}^p and $x_i \in \mathcal{X}$ denotes the design point characterizing the experimental conditions for the i -th observation Y_i , with \mathcal{X} a compact subset of \mathbb{R}^d . For the observations Y_1, \dots, Y_N performed at the design points x_1, \dots, x_N , the Least-Squares Estimator (LSE) $\hat{\theta}_{LS}^N$ is obtained by minimizing

$$S_N(\theta) = \sum_{i=1}^N [Y_i - \eta(x_i, \theta)]^2, \quad (3)$$

with respect to $\theta \in \Theta \subset \mathbb{R}^p$. We suppose throughout the paper that either the x_i 's are non-random constants or they are generated independently of the Y_j 's (i.e., the design is not sequential). We shall also use the following assumptions:

H1 $_{\eta}$: $\eta(x, \theta)$ is continuous on Θ for any $x \in \mathcal{X}$;

H2 $_{\eta}$: $\bar{\theta} \in \text{int}(\Theta)$ and $\eta(x, \theta)$ is two times continuously differentiable with respect to $\theta \in \text{int}(\Theta)$ for any $x \in \mathcal{X}$.

Then, under **H1 $_{\eta}$** the LS estimator is strongly consistent, $\hat{\theta}_{LS}^N \xrightarrow{\text{a.s.}} \bar{\theta}$, $N \rightarrow \infty$, provided that the sequence $\{x_i\}$ is "rich enough", see, e.g., [3]. For instance, when the design points form an i.i.d. sequence generated with the probability measure ξ (which is called a randomized design with measure ξ in [7, 9]), strong consistency holds under the estimability condition

$$\int_{\mathcal{X}} [\eta(x, \theta) - \eta(x, \bar{\theta})]^2 \xi(dx) = 0 \Rightarrow \theta = \bar{\theta}. \quad (4)$$

Under the additional assumption **H2 $_{\eta}$** , $\hat{\theta}_{LS}^N$ is asymptotically normally distributed,

$$\sqrt{N}(\hat{\theta}_{LS}^N - \bar{\theta}) \xrightarrow{d} z \sim \mathcal{N}(\mathbf{0}, \mathbf{M}^{-1}(\xi, \bar{\theta})), \quad N \rightarrow \infty, \quad (5)$$

provided that the information matrix (normalized, per observation)

$$\mathbf{M}(\xi, \bar{\theta}) = \frac{1}{\sigma^2} \int_{\mathcal{X}} \left. \frac{\partial \eta(x, \theta)}{\partial \theta} \right|_{\bar{\theta}} \left. \frac{\partial \eta(x, \theta)}{\partial \theta^\top} \right|_{\bar{\theta}} \xi(dx) \quad (6)$$

is nonsingular.

The paper concerns the situation where one is interested in the estimation of $h(\theta)$ rather than in the estimation of θ , with $h(\cdot)$ a continuous scalar function on Θ . Then, when the estimability condition (4) takes the relaxed form

$$\int_{\mathcal{X}} [\eta(x, \theta) - \eta(x, \bar{\theta})]^2 \xi(dx) = 0 \Rightarrow h(\theta) = h(\bar{\theta}), \quad (7)$$

we have $h(\hat{\theta}_{LS}^N) \xrightarrow{\text{a.s.}} h(\bar{\theta})$, $N \rightarrow \infty$. Under the assumption

H $_h$: $h(\theta)$ is two times continuously differentiable with respect to $\theta \in \text{int}(\Theta)$,

assuming, moreover, that $\partial h(\theta)/\partial \theta|_{\bar{\theta}} \neq \mathbf{0}$ and that (5) is satisfied, we also obtain (see [5, p. 61])

$$\sqrt{N}[h(\hat{\theta}_{LS}^N) - h(\bar{\theta})] \xrightarrow{d} \omega \sim \mathcal{N}\left(0, \left. \frac{\partial h(\theta)}{\partial \theta^\top} \right|_{\bar{\theta}} \mathbf{M}^{-1}(\xi, \bar{\theta}) \left. \frac{\partial h(\theta)}{\partial \theta} \right|_{\bar{\theta}}\right), \quad N \rightarrow \infty. \quad (8)$$

In Sect. 2 we prove a similar result on the asymptotic normality of $h(\hat{\theta}_{LS}^N)$ when $\mathbf{M}(\xi, \bar{\theta})$ is singular, that is,

$$\sqrt{N}[h(\hat{\theta}_{LS}^N) - h(\bar{\theta})] \xrightarrow{d} \omega \sim \mathcal{N}\left(0, \frac{\partial h(\theta)}{\partial \theta^\top} \Big|_{\bar{\theta}} \mathbf{M}^-(\xi, \bar{\theta}) \frac{\partial h(\theta)}{\partial \theta} \Big|_{\bar{\theta}}\right), \quad N \rightarrow \infty, \quad (9)$$

with \mathbf{M}^- a g -inverse of \mathbf{M} . This is called *regular asymptotic normality* in [9], where it is shown to hold under rather restrictive assumptions on $h(\cdot)$ but without requiring $\hat{\theta}_{LS}^N$ to be consistent. We show in Sect. 2 that when the design space \mathcal{X} is finite $\hat{\theta}_{LS}^N$ is consistent under fairly general conditions, from which (9) then easily follows.

We use the standard approach and consider an experimental design that minimizes the asymptotic variance of $h(\hat{\theta}_{LS}^N)$. According to (9), this corresponds to minimizing $[\partial h(\theta)/\partial \theta^\top |_{\bar{\theta}}] \mathbf{M}^-(\xi, \bar{\theta}) [\partial h(\theta)/\partial \theta |_{\bar{\theta}}]$. Since $\bar{\theta}$ is unknown, local c -optimal design is based on a nominal parameter value θ^0 and minimizes $\phi_c(\xi) = \Phi_c[\mathbf{M}(\xi, \theta^0)]$ with

$$\Phi_c(\cdot) : \mathbf{M} \in \mathbb{M}^{\geq} \rightarrow \begin{cases} \mathbf{c}_{\theta^0}^\top \mathbf{M}^- \mathbf{c}_{\theta^0} & \text{if and only if } \mathbf{c}_{\theta^0} \in \mathcal{M}(\mathbf{M}) \\ \infty & \text{otherwise} \end{cases} \quad (10)$$

where \mathbb{M}^{\geq} denotes the set of non-negative definite $p \times p$ matrices,

$$\mathcal{M}(\mathbf{M}) = \{\mathbf{c} : \exists \mathbf{u} \in \mathbb{R}^p, \mathbf{c} = \mathbf{M}\mathbf{u}\}$$

and

$$\mathbf{c}_{\theta^0} = \frac{\partial h(\theta)}{\partial \theta} \Big|_{\theta^0}.$$

Note that the value of $\Phi_c(\mathbf{M})$ is independent of the choice of the g -inverse \mathbf{M}^- . Nonlinearity may be present in two places, since the model response $\eta(x, \theta)$ and the function of interest $h(\theta)$ may be nonlinear in θ . Local c -optimal design corresponds to c -optimal design in the linear (or more precisely linearized) model $\eta_L(x, \theta) = \mathbf{f}_{\theta^0}^\top(x)\theta$ where $\mathbf{f}_{\theta^0}(x) = \partial \eta(x, \theta)/\partial \theta |_{\theta^0}$, with the linear (linearized) function of interest $h_L(\theta) = \mathbf{c}_{\theta^0}^\top \theta$. A design ξ^* minimizing $\phi_c(\xi)$ may be singular, in the sense that the matrix $\mathbf{M}(\xi^*, \theta^0)$ is singular. In spite of an apparent simplicity for linear models, this yields, however, a difficulty due to the fact that the function $\Phi_c(\cdot)$ is only lower semi-continuous at a singular matrix $\mathbf{M} \in \mathbb{M}^{\geq}$. Indeed, this property implies that

$$\lim_{N \rightarrow \infty} \mathbf{c}^\top \mathbf{M}^-(\xi_N) \mathbf{c} \geq \mathbf{c}^\top \mathbf{M}^-(\xi) \mathbf{c}$$

when the empirical measure ξ_N of the design points converges weakly to ξ , see e.g. [6, p. 67] and [8] for examples with strict inequality. The two types of nonlinearities mentioned above cause additional difficulties in the presence of a singular design: both $\hat{\theta}_{LS}^N$ and $h(\hat{\theta}_{LS}^N)$ may not be consistent, or the asymptotic normality (9) may not hold, see [8] for an example with a linear model and a nonlinear function $h(\cdot)$. It is the purpose of the paper to expose some of those difficulties and to make suggestions for regularizing a singular c -optimal design.

2 Asymptotic properties of LSE with finite \mathcal{X}

When using a sequence of design points i.i.d. with the measure ξ , the condition (4) implies that $S_N(\theta)$ given by (3) grows to infinity at rate N when $\theta \neq \bar{\theta}$ (an assumption used in the classic reference [3]). On the other hand, for a design sequence with associated empirical measure converging to a discrete measure ξ , this amounts to ignoring the information provided by design points $x \in \mathcal{X}$ with a relative frequency $r_N(x)/N$ tending to zero, which therefore do not appear in the support of ξ . In order to acknowledge the information carried by such points, we can follow the same approach as in [10] from which we extract the following lemma.

Lemma 1 *If for any $\delta > 0$*

$$\liminf_{N \rightarrow \infty} \inf_{\|\theta - \bar{\theta}\| \geq \delta} [S_N(\theta) - S_N(\bar{\theta})] > 0 \text{ a.s.} \quad (11)$$

then $\hat{\theta}_{LS}^N \xrightarrow{\text{a.s.}} \bar{\theta}$ as $N \rightarrow \infty$. If for any $\delta > 0$

$$\Pr \left\{ \inf_{\|\theta - \bar{\theta}\| \geq \delta} [S_N(\theta) - S_N(\bar{\theta})] > 0 \right\} \rightarrow 1, \quad N \rightarrow \infty, \quad (12)$$

then $\hat{\theta}_{LS}^N \xrightarrow{\text{P}} \bar{\theta}$ as $N \rightarrow \infty$.

We can then prove the convergence of the LS estimator (in probability and a.s.) when the sum $\sum_{k=1}^N [\eta(x_k, \theta) - \eta(x_k, \bar{\theta})]^2$ tends to infinity fast enough for $\|\theta - \bar{\theta}\| \geq \delta > 0$ and the design space \mathcal{X} for the x_k 's is finite.

Theorem 1 *Let $\{x_i\}$ be a design sequence on a finite set \mathcal{X} . If $D_N(\theta, \bar{\theta}) = \sum_{k=1}^N [\eta(x_k, \theta) - \eta(x_k, \bar{\theta})]^2$ satisfies*

$$\text{for all } \delta > 0, \quad \left[\inf_{\|\theta - \bar{\theta}\| \geq \delta} D_N(\theta, \bar{\theta}) \right] / (\log \log N) \rightarrow \infty, \quad N \rightarrow \infty, \quad (13)$$

then $\hat{\theta}_{LS}^N \xrightarrow{\text{a.s.}} \bar{\theta}$ as $N \rightarrow \infty$. If $D_N(\theta, \bar{\theta})$ simply satisfies

$$\text{for all } \delta > 0, \quad \inf_{\|\theta - \bar{\theta}\| \geq \delta} D_N(\theta, \bar{\theta}) \rightarrow \infty \text{ as } N \rightarrow \infty, \quad (14)$$

then $\hat{\theta}_{LS}^N \xrightarrow{\text{P}} \bar{\theta}$, $N \rightarrow \infty$.

Proof. The proof is based on Lemma 1. We have

$$\begin{aligned} S_N(\theta) - S_N(\bar{\theta}) &= D_N(\theta, \bar{\theta}) \left[1 + 2 \frac{\sum_{x \in \mathcal{X}} \left(\sum_{k=1, x_k=x}^N \varepsilon_k \right) [\eta(x, \bar{\theta}) - \eta(x, \theta)]}{D_N(\theta, \bar{\theta})} \right] \\ &\geq D_N(\theta, \bar{\theta}) \left[1 - 2 \frac{\sum_{x \in \mathcal{X}} \left| \sum_{k=1, x_k=x}^N \varepsilon_k \right| |\eta(x, \bar{\theta}) - \eta(x, \theta)|}{D_N(\theta, \bar{\theta})} \right]. \end{aligned}$$

From Lemma 1, under the condition (13) it suffices to prove that

$$\sup_{\|\theta - \bar{\theta}\| \geq \delta} \frac{\sum_{x \in \mathcal{X}} \left| \sum_{k=1, x_k=x}^N \varepsilon_k \right| |\eta(x, \bar{\theta}) - \eta(x, \theta)|}{D_N(\theta, \bar{\theta})} \xrightarrow{\text{a.s.}} 0 \quad (15)$$

for any $\delta > 0$ to obtain the strong consistency of $\hat{\theta}_{LS}^N$. Since $D_N(\theta, \bar{\theta}) \rightarrow \infty$ and \mathcal{X} is finite, only the design points such that $r_N(x) \rightarrow \infty$ have to be considered, where $r_N(x)$ denotes the number of times x appears in the sequence x_1, \dots, x_N . Define $\beta(n) = \sqrt{n \log \log n}$. From the law of the iterated logarithm,

$$\text{for all } x \in \mathcal{X}, \quad \limsup_{r_N(x) \rightarrow \infty} \left| \frac{1}{\beta[r_N(x)]} \sum_{k=1, x_k=x}^N \varepsilon_k \right| = \sigma\sqrt{2}, \quad \text{almost surely.} \quad (16)$$

Moreover, $D_N(\theta, \bar{\theta}) \geq D_N^{1/2}(\theta, \bar{\theta}) \sqrt{r_N(x)} |\eta(x, \bar{\theta}) - \eta(x, \theta)|$ for any $x \in \mathcal{X}$, so that

$$\frac{\beta[r_N(x)] |\eta(x, \bar{\theta}) - \eta(x, \theta)|}{D_N(\theta, \bar{\theta})} \leq \frac{[\log \log r_N(x)]^{1/2}}{D_N^{1/2}(\theta, \bar{\theta})}.$$

Therefore,

$$\frac{\left| \sum_{k=1, x_k=x}^N \varepsilon_k \right| |\eta(x, \bar{\theta}) - \eta(x, \theta)|}{D_N(\theta, \bar{\theta})} \leq \left| \frac{\sum_{k=1, x_k=x}^N \varepsilon_k}{\beta[r_N(x)]} \right| \frac{[\log \log r_N(x)]^{1/2}}{D_N^{1/2}(\theta, \bar{\theta})},$$

which, together with (13) and (16), gives (15).

When $\inf_{\|\theta - \bar{\theta}\| \geq \delta} D_N(\theta, \bar{\theta}) \rightarrow \infty$ as $N \rightarrow \infty$, we only need to prove that

$$\sup_{\|\theta - \bar{\theta}\| \geq \delta} \frac{\sum_{x \in \mathcal{X}} \left| \sum_{k=1, x_k=x}^N \varepsilon_k \right| |\eta(x, \bar{\theta}) - \eta(x, \theta)|}{D_N(\theta, \bar{\theta})} \xrightarrow{P} 0 \quad (17)$$

for any $\delta > 0$ to obtain the weak consistency of $\hat{\theta}_{LS}^N$. We proceed as above and only consider the design points such that $r_N(x) \rightarrow \infty$, with now $\beta(n) = \sqrt{n}$. From the central limit theorem, for any $x \in \mathcal{X}$, $\left(\sum_{k=1, x_k=x}^N \varepsilon_k \right) / \sqrt{r_N(x)} \xrightarrow{d} \omega_x \sim \mathcal{N}(0, \sigma^2)$ as $r_N(x) \rightarrow \infty$ and is thus bounded in probability. Also, for any $x \in \mathcal{X}$, $\sqrt{r_N(x)} |\eta(x, \bar{\theta}) - \eta(x, \theta)| / D_N(\theta, \bar{\theta}) \leq D_N^{-1/2}(\theta, \bar{\theta})$, so that (14) implies (17). \blacksquare

When the design space \mathcal{X} is finite one can thus invoke Theorem 1 to ensure the consistency of $\hat{\theta}_{LS}^N$. Regular asymptotic normality then follows for suitable functions $h(\cdot)$.

Theorem 2 *Let $\{x_i\}$ be a design sequence on a finite set \mathcal{X} , with the property that the associated empirical measure (strongly) converges to ξ (possibly singular), that is, $\lim_{N \rightarrow \infty} r_N(x)/N = \xi(x)$ for any $x \in \mathcal{X}$, with $r_N(x)$ the number of*

times x appears in the sequence x_1, \dots, x_N . Suppose that the assumptions $\mathbf{H1}_\eta$, $\mathbf{H2}_\eta$ and \mathbf{H}_h are satisfied, with $\partial h(\theta)/\partial\theta|_{\bar{\theta}} \neq \mathbf{0}$, and that $D_N(\theta, \bar{\theta})$ satisfies (13). Then,

$$\left. \frac{\partial h(\theta)}{\partial\theta} \right|_{\bar{\theta}} \in \mathcal{M}[\mathbf{M}(\xi, \bar{\theta})], \quad (18)$$

implies that $h(\hat{\theta}_{LS}^N)$ satisfies the regular asymptotic normality property (9), where the choice of the g -inverse is arbitrary.

Proof. Since $\hat{\theta}_{LS}^N \xrightarrow{\text{a.s.}} \bar{\theta} \in \text{int}(\Theta)$, there exists N_0 such that $\hat{\theta}_{LS}^N$ is in some convex neighborhood of $\bar{\theta}$ for all N larger than N_0 and, for all $i = 1, \dots, p = \dim(\theta)$, a Taylor development of the i -th component of the gradient of the LS criterion (3) gives

$$\{\nabla_\theta S_N(\hat{\theta}_{LS}^N)\}_i = 0 = \{\nabla_\theta S_N(\bar{\theta})\}_i + \{\nabla_\theta^2 S_N(\beta_i^N)(\hat{\theta}_{LS}^N - \bar{\theta})\}_i, \quad (19)$$

with β_i^N between $\hat{\theta}_{LS}^N$ and $\bar{\theta}$ (and β_i^N measurable, see [3]). Using the fact that \mathcal{X} is finite we obtain $\nabla_\theta S_N(\bar{\theta})/\sqrt{N} \xrightarrow{\text{d}} \mathbf{v} \sim \mathcal{N}(\mathbf{0}, 4\mathbf{M}(\xi, \bar{\theta}))$ and $\nabla_\theta^2 S_N(\beta_i^N)/N \xrightarrow{\text{a.s.}} 2\mathbf{M}(\xi, \bar{\theta})$ as $N \rightarrow \infty$. Combining this with (19), we get

$$\sqrt{N}\mathbf{c}^\top \mathbf{M}(\xi, \bar{\theta})(\hat{\theta}_{LS}^N - \bar{\theta}) \xrightarrow{\text{d}} z \sim \mathcal{N}(0, \mathbf{c}^\top \mathbf{M}(\xi, \bar{\theta})\mathbf{c}), \quad N \rightarrow \infty,$$

for any $\mathbf{c} \in \mathbb{R}^p$. Applying the Taylor formula again we can write

$$\sqrt{N}[h(\hat{\theta}_{LS}^N) - h(\bar{\theta})] = \sqrt{N} \left. \frac{\partial h(\theta)}{\partial\theta^\top} \right|_{\alpha^N} (\hat{\theta}_{LS}^N - \bar{\theta})$$

for some α^N between $\hat{\theta}_{LS}^N$ and $\bar{\theta}$ and $\partial h(\theta)/\partial\theta|_{\alpha^N} \xrightarrow{\text{a.s.}} \partial h(\theta)/\partial\theta|_{\bar{\theta}}$ as $N \rightarrow \infty$. When (18) is satisfied we can write $\partial h(\theta)/\partial\theta|_{\bar{\theta}} = \mathbf{M}(\xi, \bar{\theta})\mathbf{u}$ for some $\mathbf{u} \in \mathbb{R}^p$, which gives (9). \blacksquare

Notice that when $\mathbf{M}(\xi, \bar{\theta})$ has full rank the condition (18) is automatically satisfied so that the other conditions of Theorem 2 are sufficient for the asymptotic normality (8). The conclusion of the Theorem remains valid when $D_N(\theta, \bar{\theta})$ only satisfies (14) (convergence in probability of $\hat{\theta}_{LS}^N$) with Θ a convex set, see, e.g., [1, Th. 4.2.2].

3 Properties of standard regularization

Consider a regularized version of the c -optimality criterion defined by

$$\Phi_c^\gamma(\mathbf{M}) = \Phi_c[(1 - \gamma)\mathbf{M} + \gamma\tilde{\mathbf{M}}]$$

with $\Phi_c(\cdot)$ given by (10), γ a small positive number and $\tilde{\mathbf{M}}$ a fixed nonsingular $p \times p$ matrix of \mathbb{M}^\geq . From the linearity of $\mathbf{M}(\xi, \theta^0)$ in ξ , when $\tilde{\mathbf{M}} = \mathbf{M}(\xi, \theta^0)$ with $\tilde{\xi}$ nonsingular this equivalently defines the criterion

$$\phi_c^\gamma(\xi) = \phi_c[(1 - \gamma)\xi + \gamma\tilde{\xi}]$$

with $\phi_c(\xi) = \Phi_c[\mathbf{M}(\xi, \theta^0)]$. Let ξ^* and ξ_γ^* be two measures respectively optimal for $\phi_c(\cdot)$ and $\phi_c^\gamma(\cdot)$. We have $\phi_c(\xi^*) \leq \phi_c[(1-\gamma)\xi_\gamma^* + \gamma\tilde{\xi}] = \phi_c^\gamma(\xi_\gamma^*) \leq \phi_c[(1-\gamma)\xi^* + \gamma\tilde{\xi}] \leq (1-\gamma)\phi_c(\xi^*) + \gamma\phi_c(\tilde{\xi})$, where the last inequality follows from the convexity of $\phi_c(\cdot)$. Therefore,

$$0 \leq \phi_c^\gamma(\xi_\gamma^*) - \phi_c(\xi^*) \leq \gamma[\phi_c(\tilde{\xi}) - \phi_c(\xi^*)]$$

which tends to zero as $\gamma \rightarrow 0$, showing that $\hat{\xi}_\gamma = (1-\gamma)\xi_\gamma^* + \gamma\tilde{\xi}$ tends to be c -optimal when γ decreases to zero.

We emphasize that c -optimality is defined for $\theta^0 \neq \bar{\theta}$. Let $x^{(1)}, \dots, x^{(s)}$ be the support points of a c -optimal measure ξ^* , complement them by $x^{(s+1)}, \dots, x^{(s+k)}$ so that the measure $\tilde{\xi}$ supported at $x^{(1)}, \dots, x^{(s+k)}$ (with, e.g., equal weight at each point) is nonsingular. When N observations are made, the measure $(1-\gamma)\xi^* + \gamma\tilde{\xi}$ corresponds a design that places approximately $\gamma N/(s+k)$ observations at each of the points $x^{(s+1)}, \dots, x^{(s+k)}$. The example below shows that the speed of convergence of $\mathbf{c}^\top \hat{\theta}_{LS}^N$ to $\mathbf{c}^\top \bar{\theta}$ may be arbitrarily slow when γ tends to zero, thereby contradicting the acceptance of ξ^* as a c -optimal design for $\bar{\theta}$.

Example: Consider the regression model defined by (1,2) with

$$\eta(x, \theta) = \frac{\theta_1}{\theta_1 - \theta_2} [\exp(-\theta_2 x) - \exp(-\theta_1 x)],$$

$\mathcal{X} = [0, 10]$ and $\sigma^2 = 1$. The D -optimal design measure ξ_D^* on \mathcal{X} maximizing $\log \det \mathbf{M}(\xi, \theta^0)$ for the nominal parameters $\theta^0 = (0.7, 0.2)^\top$ puts mass 1/2 at each of the two support points given approximately by $x^{(1)} = 1.25$, $x^{(2)} = 6.60$.

Figure 1 shows the set $\{\mathbf{f}_{\theta^0}(x) : x \in \mathcal{X}\}$ (solid line), its symmetric $\{-\mathbf{f}_{\theta^0}(x) : x \in \mathcal{X}\}$ (dashed line) and their convex closure \mathcal{F}_{θ^0} , called the Elfving set (shaded region), together with the minimum-volume ellipsoid containing \mathcal{F}_{θ^0} (the points of contact with \mathcal{F}_{θ^0} correspond to the support points of ξ_D^*).

From Elfving's theorem [2], when $x^* \in [x^{(1)}, x^{(2)}]$ the c -optimal design minimizing $\mathbf{c}^\top \mathbf{M}^{-1}(\xi, \theta^0) \mathbf{c}$ with $\mathbf{c} = \beta \mathbf{f}_{\theta^0}(x_*)$, $\beta \neq 0$, is the delta measure δ_{x^*} . Obviously, the singular design δ_{x^*} only allows us to estimate $\eta(x_*, \theta)$ and not $h(\theta) = \mathbf{c}^\top \theta$.

Select now a second design point $x^0 \neq x_*$ and suppose that when N observations are performed at the design points x_1, \dots, x_N , m of them coincide with x^0 and $N - m$ with x_* , where $m/(\log \log N) \rightarrow \infty$ with $m/N \rightarrow 0$. Then, for $x^0 \neq 0$ the conditions of Theorem 1 are satisfied. Indeed, the design space equals $\{x^0, x_*\}$ and is thus finite, and

$$\begin{aligned} D_N(\theta, \bar{\theta}) &= \sum_{k=1}^N [\eta(x_k, \theta) - \eta(x_k, \bar{\theta})]^2 \\ &= (N - 2m)[\eta(x_*, \theta) - \eta(x_*, \bar{\theta})]^2 \\ &\quad + m \{ [\eta(x_*, \theta) - \eta(x_*, \bar{\theta})]^2 + [\eta(x^0, \theta) - \eta(x^0, \bar{\theta})]^2 \} \end{aligned}$$

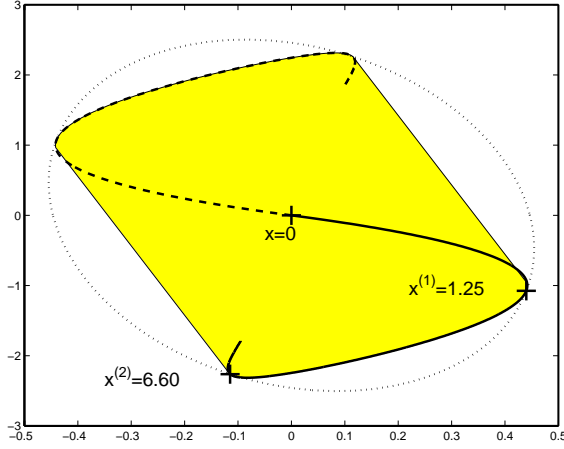


Figure 1: Elfving set.

so that $\inf_{\|\theta - \bar{\theta}\| > \delta} D_N(\theta, \bar{\theta}) \geq mC(x^0, x_*, \delta)$, with $C(x^0, x_*, \delta)$ a positive constant, and $\inf_{\|\theta - \bar{\theta}\| > \delta} D_N(\theta, \bar{\theta}) / (\log \log N) \rightarrow \infty$ as $N \rightarrow \infty$. Therefore, although the empirical measure ξ_N of the design points in the experiment converges strongly to the singular design δ_{x_*} , this convergence is sufficiently slow to make $\hat{\theta}_{LS}^N$ (strongly) consistent. Moreover, for $h(\cdot)$ a function satisfying the conditions of Theorem 2, $h(\hat{\theta}_{LS}^N)$ satisfies the regular asymptotic property (9). In the present situation, this means that when $\partial h(\theta) / \partial \theta|_{\bar{\theta}} = \beta \mathbf{f}_{\bar{\theta}}(x_*)$ for some $\beta \in \mathbb{R}$, then $\sqrt{N}[h(\hat{\theta}_{LS}^N) - h(\bar{\theta})] \xrightarrow{d} \omega \sim \mathcal{N}(0, [\partial h(\theta) / \partial \theta]^\top \mathbf{M}^-(\delta_{x_*}, \theta) \partial h(\theta) / \partial \theta|_{\bar{\theta}})$. This holds for instance when $h(\cdot) = \eta(x_*, \cdot)$ (or is a function of $\eta(x_*, \cdot)$).

There is, however, a severe limitation in the application of this result in practical situations. Indeed, the direction $\mathbf{f}_{\bar{\theta}}(x_*)$ for which regular asymptotic normality holds is unknown since $\bar{\theta}$ is unknown. Let \mathbf{c} be a given direction of interest, the associated c -optimal design ξ^* is determined for the nominal value θ^0 . For instance, when $\mathbf{c} = (0, 1)^\top$ (which means that one is only interested in the estimation of the component θ_2), $\xi^* = \delta_{x_*}$ with x_* solution of $\{\mathbf{f}_{\theta^0}(x)\}_1 = 0$ (see Figure 1), that is, x_* satisfies

$$\theta_2^0 = [\theta_2^0 + \theta_1^0(\theta_1^0 - \theta_2^0)x_*] \exp[-(\theta_1^0 - \theta_2^0)x_*]. \quad (20)$$

For $\theta^0 = (0.7, 0.2)^\top$, this gives $x_* = x_*(\theta^0) \simeq 4.28$. In general, $\mathbf{f}_{\bar{\theta}}(x_*) \neq \mathbf{f}_{\theta^0}(x_*)$ to which \mathbf{c} is proportional. Therefore, $\mathbf{c} \notin \mathcal{M}[\mathbf{M}(\xi^*, \bar{\theta})]$ and regular asymptotic normality does not hold for $\mathbf{c}^\top \hat{\theta}_{LS}^N$.

The example is simple enough to be able to investigate the limiting behavior of $\mathbf{c}^\top \hat{\theta}_{LS}^N$ by direct calculation. A Taylor development of the LS criterion $S_N(\theta)$ gives (19) where $\beta_i^N \xrightarrow{\text{a.s.}} \bar{\theta}$ as $N \rightarrow \infty$, $i = 1, 2$. Direct calculations give

$$\begin{aligned} \nabla_{\theta} S_N(\bar{\theta}) &= -2 \left[\sqrt{m} \beta_m \mathbf{f}_{\bar{\theta}}(x^0) + \sqrt{N-m} \gamma_{N-m} \mathbf{f}_{\bar{\theta}}(x_*) \right], \\ \nabla_{\theta}^2 S_N(\bar{\theta}) &= 2 \left[m \mathbf{f}_{\bar{\theta}}(x^0) \mathbf{f}_{\bar{\theta}}^\top(x^0) + (N-m) \mathbf{f}_{\bar{\theta}}(x_*) \mathbf{f}_{\bar{\theta}}^\top(x_*) \right] + \mathcal{O}_p(\sqrt{m}), \end{aligned}$$

where $\beta_m = (1/\sqrt{m}) \sum_{x_i=x^0} \varepsilon_i$ and $\gamma_{N-m} = (1/\sqrt{N-m}) \sum_{x_i=x_*} \varepsilon_i$ are independent random variables that tend to be distributed $\mathcal{N}(0, 1)$ as $m \rightarrow \infty$ and $N - m \rightarrow \infty$. We then obtain,

$$\hat{\theta}_{LS}^N - \bar{\theta} = \frac{1}{\Delta(x_*, x^0)} \left\{ \frac{\gamma_{N-m}}{\sqrt{N-m}} \begin{pmatrix} \{\mathbf{f}_{\bar{\theta}}(x^0)\}_2 \\ -\{\mathbf{f}_{\bar{\theta}}(x^0)\}_1 \end{pmatrix} + \frac{\beta_m}{\sqrt{m}} \begin{pmatrix} -\{\mathbf{f}_{\bar{\theta}}(x_*)\}_2 \\ \{\mathbf{f}_{\bar{\theta}}(x_*)\}_1 \end{pmatrix} \right\} + o_p(1/\sqrt{m}),$$

where $\Delta(x_*, x^0) = \det(\mathbf{f}_{\bar{\theta}}(x_*), \mathbf{f}_{\bar{\theta}}(x^0))$. Therefore, $\sqrt{N} \mathbf{f}_{\bar{\theta}}^\top(x_*) (\hat{\theta}_{LS}^N - \bar{\theta})$ is asymptotically normal $\mathcal{N}(0, 1)$ whereas for any direction \mathbf{c} not parallel to $\mathbf{f}_{\bar{\theta}}(x_*)$ and not orthogonal to $\mathbf{f}_{\bar{\theta}}(x^0)$, $\sqrt{m} \mathbf{c}^\top (\hat{\theta}_{LS}^N - \bar{\theta})$ is asymptotically normal (and $\mathbf{c}^\top (\hat{\theta}_{LS}^N - \bar{\theta})$ converges not faster than $1/\sqrt{m}$). In particular, $\sqrt{m} \mathbf{f}_{\bar{\theta}}^\top(x^0) (\hat{\theta}_{LS}^N - \bar{\theta})$ is asymptotically normal $\mathcal{N}(0, 1)$ and $\sqrt{m} \{\hat{\theta}_{LS}^N - \bar{\theta}\}_2$ is asymptotically normal $\mathcal{N}(0, \{\mathbf{f}_{\bar{\theta}}(x_*)\}_1^2 / \Delta^2(x_*, x^0))$. \square

The previous example has illustrated that letting γ tend to zero in a regularized c -optimal design $(1-\gamma)\xi^* + \gamma\tilde{\xi}$ raises important difficulties (one may refer to [8] for an example with a linear model and a nonlinear function $h(\theta)$). We shall therefore consider γ as fixed in what follows. It is interesting, nevertheless, to investigate the behavior of the c -optimality criterion when the regularized measure $(1-\gamma)\xi^* + \gamma\tilde{\xi}$ approaches ξ^* in some sense. Since γ is now fixed, we let the support points of $\tilde{\xi}$ approach those of ξ^* . This is illustrated by continuing the example above.

Example (continued): Place the proportion $m = N/2$ of the observations at x^0 and consider the design measure $\xi_{\gamma, x^0} = (1-\gamma)\delta_{x_*} + \gamma\delta_{x^0}$ with $\gamma = 1/2$. Since the c -optimal design is δ_{x_*} , we consider the limiting behavior of $\mathbf{c}^\top (\hat{\theta}_{LS}^N - \bar{\theta})$ when N tends to infinity for x^0 approaching x_* . The nonsingularity of $\xi_{1/2, x^0}$ for $x^0 \neq x_*$ (and $x^0 \neq 0$) implies that $\sqrt{N} \mathbf{c}^\top (\hat{\theta}_{LS}^N - \bar{\theta})$ is asymptotically normal $\mathcal{N}(0, \mathbf{c}^\top \mathbf{M}^{-1}(\xi_{1/2, x^0}, \bar{\theta}) \mathbf{c})$.

The asymptotic variance $\mathbf{c}^\top \mathbf{M}^{-1}(\xi_{1/2, x^0}, \bar{\theta}) \mathbf{c}$ tends to infinity as x^0 tends to x_* when \mathbf{c} is not proportional to $\mathbf{f}_{\bar{\theta}}(x_*)$, see Figure 2. Take $\mathbf{c} = \mathbf{f}_{\bar{\theta}}(x_*)$. Then, $\mathbf{f}_{\bar{\theta}}^\top(x_*) \mathbf{M}^{-1}(\xi_{1/2, x^0}, \bar{\theta}) \mathbf{f}_{\bar{\theta}}(x_*)$ equals 2 for any $x^0 \neq x_*$, twice more than what could be achieved with the singular design δ_{x_*} since $\mathbf{f}_{\bar{\theta}}^\top(x_*) \mathbf{M}^{-1}(\delta_{x_*}, \bar{\theta}) \mathbf{f}_{\bar{\theta}}(x_*) = 1$ (this result is similar to that in [6, p. 67] and is caused by the fact that $\Phi_c(\cdot)$ is only semi-continuous at a singular \mathbf{M}). \square

The example above shows that not all regularizations are legitimate: the regularized design should be close to the optimal one ξ^* in some suitable sense in order to avoid the discontinuity of $\Phi_c(\cdot)$ at a singular \mathbf{M} .

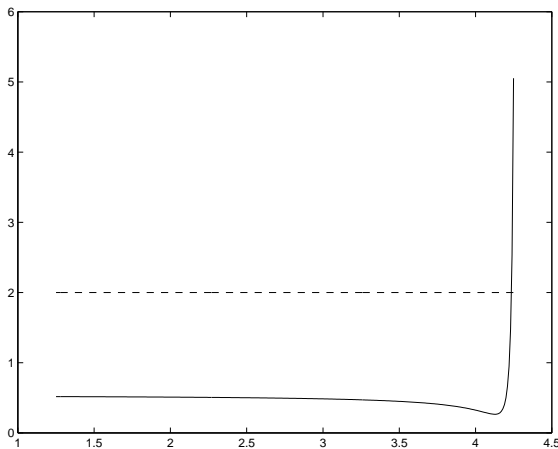


Figure 2: $\mathbf{c}^\top \mathbf{M}^{-1}(\xi_{1/2, x^0}, \bar{\theta}) \mathbf{c}$ (solid line) and $\mathbf{f}_{\bar{\theta}}^\top(x_*) \mathbf{M}^{-1}(\xi_{1/2, x^0}, \bar{\theta}) \mathbf{f}_{\bar{\theta}}(x_*)$ (dashed line) for x^0 varying between 1.25 and $x_* = 4.28$; $\bar{\theta} = (0.65, 0.25)^\top$, $\theta^0 = (0.7, 0.2)^\top$ and $\mathbf{c} = (0, 1)^\top$ (so that δ_{x_*} is c -optimal for \mathbf{c} and θ^0).

4 Minimax regularization

4.1 Estimation of a nonlinear function of θ

Consider first the case where the function of interest $h(\theta)$ is nonlinear in θ . We should then ideally take $\mathbf{c}_{\bar{\theta}} = \partial h(\theta) / \partial \theta|_{\bar{\theta}}$ in the definition of the optimality criterion. However, since $\bar{\theta}$ is unknown, a direct application of local c -optimal design consists in using the direction $\mathbf{c}_{\theta^0} = \partial h(\theta) / \partial \theta|_{\theta^0}$, with the risk that θ and $h(\theta)$ are not estimable from the associated optimal design ξ^* if it is singular. One can then consider instead a set Θ^0 (a finite set or a compact subset of \mathbb{R}^p) of possible values for $\bar{\theta}$ around θ^0 in the definition of the directions of interest, and the associated c -minimax optimality criterion becomes

$$\phi_{\mathcal{C}}(\xi) = \max_{\theta \in \Theta^0} \mathbf{c}_{\theta}^\top \mathbf{M}^{-1}(\xi, \theta^0) \mathbf{c}_{\theta}, \quad (21)$$

or equivalently $\phi_{\mathcal{C}}(\xi) = \max_{\mathbf{c} \in \mathcal{C}} \mathbf{c}^\top \mathbf{M}^{-1}(\xi, \theta^0) \mathbf{c}$ with $\mathcal{C} = \{\mathbf{c}_{\theta} : \theta \in \Theta^0\}$. A measure $\xi^*(\mathcal{C})$ on \mathcal{X} that minimizes $\phi_{\mathcal{C}}(\xi)$ is said to be (locally) c -minimax optimal. When \mathcal{C} is large enough (in particular when the vectors in \mathcal{C} span \mathbb{R}^p), $\xi^*(\mathcal{C})$ is nonsingular. According to Theorem 2, a design sequence on a finite set \mathcal{X} (containing the support of $\xi^*(\mathcal{C})$) such that the associated empirical measure converges strongly to $\xi^*(\mathcal{C})$ then ensures the asymptotic normality property (8).

4.2 Estimation of a linear function of θ : regularization via D -optimal design

When the function of interest is $h(\theta) = \mathbf{c}^\top \theta$ with the direction \mathbf{c} fixed, the construction of an admissible set \mathcal{C} of directions for c -minimax optimal design

is somewhat artificial and a specific procedure is required. The rest of the section is devoted to this situation. The first approach presented is based on D -optimality and applies when the c -optimal measure is a one-point measure.

Define a (local) c -maximin efficient measure ξ_{mm}^* for \mathcal{C} as a measure on \mathcal{X} that maximizes

$$E_{mm}(\xi) = \min_{\mathbf{c} \in \mathcal{C}} \frac{\mathbf{c}^\top \mathbf{M}^{-1}[\xi^*(\mathbf{c}), \theta^0] \mathbf{c}}{\mathbf{c}^\top \mathbf{M}^{-1}(\xi, \theta^0) \mathbf{c}},$$

with $\xi^*(\mathbf{c})$ a c -optimal design measure minimizing $\mathbf{c}^\top \mathbf{M}^{-1}(\xi, \theta^0) \mathbf{c}$. When the c -optimal design $\xi^*(\mathbf{c})$ is the delta measure δ_{x^*} it seems reasonable to consider measures that are supported in the neighborhood of x^* . One may then use the following result of Kiefer [4] to obtain a c -maximin efficient measure through D -optimal design.

Theorem 3 *A design measure ξ_{mm}^* on \mathcal{X} is c -maximin efficient for $\mathcal{C}_\mathcal{X} = \{\mathbf{f}_{\theta^0}(x) : x \in \mathcal{X}\}$ if and only if it is D -optimal on \mathcal{X} , that is, it maximizes $\log \det \mathbf{M}(\xi, \theta^0)$.*

The construction is as follows. Define

$$\mathcal{X}_\delta = \mathcal{B}(x_*, \delta) \cap \mathcal{X}, \quad (22)$$

with $\mathcal{B}(x_*, \delta)$ the ball of centre x_* and radius δ in \mathbb{R}^d , and define $\mathcal{C}_\delta = \{\mathbf{f}_{\theta^0}(x) : x \in \mathcal{X}_\delta\}$. From Theorem 3, a measure ξ_δ^* is c -maximin efficient for $\mathbf{c} \in \mathcal{C}_\delta$ if and only if it is D -optimal on \mathcal{X}_δ . Suppose that \mathcal{C}_δ spans \mathbb{R}^p when $\delta > 0$, the measure ξ_δ^* is then non singular for $\delta > 0$ (with $\xi_0^* = \xi^*(\mathbf{c})$). Various values of δ are associated with different designs ξ_δ^* . One may then choose δ by minimizing

$$J(\delta) = \max_{\theta \in \Theta^0} \Phi_c[\mathbf{M}(\xi_\delta^*, \theta)], \quad (23)$$

where Θ^0 defines a feasible set for the unknown parameter vector $\bar{\theta}$. Each evaluation of $J(\delta)$ requires the determination of a D -optimal design on a set \mathcal{X}_δ and the determination of the minimum with respect to $\theta \in \Theta^0$, but the D -optimal design is often easily obtained, see the example below, and the set Θ^0 can be discretized to facilitate the determination of the maximum.

Example (continued): Take $\mathbf{c} = (0, 1)^\top$ and $\theta^0 = (0.7, 0.2)^\top$. Choosing \mathcal{X}_δ as in (22) gives $\mathcal{C}_\delta = \{\mathbf{f}_{\theta^0}(x) : x \in [x_* - \delta, x_* + \delta]\}$, with $x_* \simeq 4.28$, and the corresponding c -maximin efficient measure is $\xi_\delta^* = (1/2)\delta_{x_* - \delta} + (1/2)\delta_{x_* + \delta}$. Fig. 3 shows $\mathbf{c}^\top \mathbf{M}^{-1}(\xi_\delta^*, \bar{\theta}) \mathbf{c}$ and $\mathbf{f}_{\bar{\theta}}^\top(x_*) \mathbf{M}^{-1}(\xi_\delta^*, \bar{\theta}) \mathbf{f}_{\bar{\theta}}(x_*)$ as functions of δ . Notice that $\mathbf{f}_{\bar{\theta}}^\top(x_*) \mathbf{M}^{-1}(\xi_\delta^*, \bar{\theta}) \mathbf{f}_{\bar{\theta}}(x_*)$ tends to 1 as δ tends to zero, indicating that the form of the neighborhood used in the construction of \mathcal{X}_δ has a strong influence on the performance of ξ_δ^* (in terms of c -optimality) when δ tends to zero. Indeed, taking $\mathcal{X}_\delta = [x^0, x_*]$ with $x^0 = x_* - \delta$ yields the same situation as that depicted in Fig. 2.

The curve showing $\mathbf{c}^\top \mathbf{M}^{-1}(\xi_\delta^*, \bar{\theta}) \mathbf{c}$ in Fig. 3 indicates the presence of a minimum around $\delta = 0.5$. Fig. 4 presents $J(\delta)$ given by (23) as a function of δ when $\Theta^0 = [0.6, 0.8] \times [0.1, 0.3]$, indicating a minimum around $\delta = 1.45$ (the maximum over θ is attained at the endpoints $\theta_1 = 0.8, \theta_2 = 0.3$ for any δ). \square

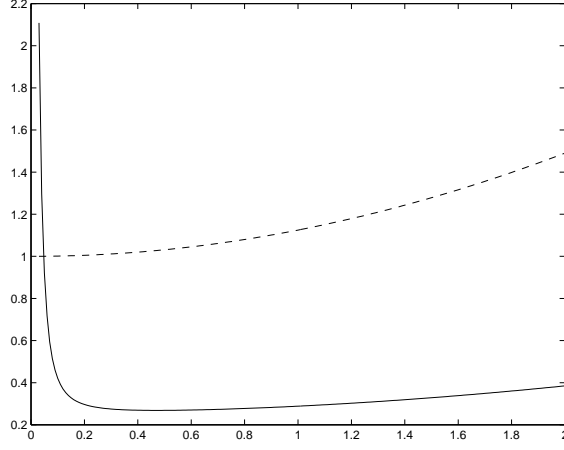


Figure 3: $\mathbf{c}^\top \mathbf{M}^{-1}(\xi_\delta^*, \bar{\theta}) \mathbf{c}$ (solid line) and $\mathbf{f}_\theta^\top(x_*) \mathbf{M}^{-1}(\xi_\delta^*, \bar{\theta}) \mathbf{f}_\theta(x_*)$ (dashed line) for δ between 0 and 2; $x_* = 4.28$, $\bar{\theta} = (0.65, 0.25)^\top$, $\theta^0 = (0.7, 0.2)^\top$ and $\mathbf{c} = (0, 1)^\top$ (so that δ_{x_*} is c -optimal for \mathbf{c} and θ^0).

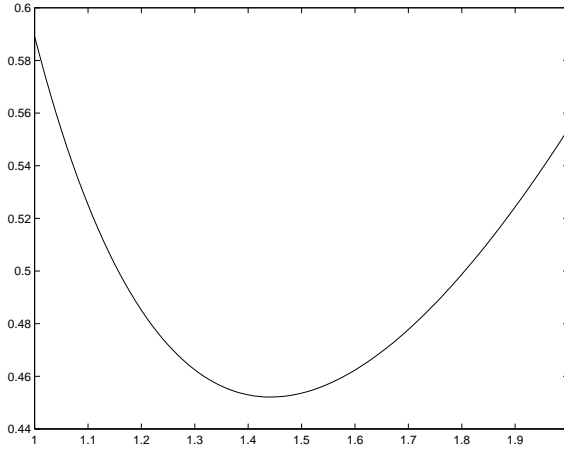


Figure 4: $\max_{\theta \in \Theta^0} \mathbf{c}^\top \mathbf{M}^{-1}(\xi_\delta^*, \theta) \mathbf{c}$ as a function of $\delta \in [1, 2]$ for $\Theta^0 = [0.6, 0.8] \times [0.1, 0.3]$.

5 Regularization by combination of c -optimal designs

We say that $h(\theta)$ is *locally estimable* at θ for the design ξ in the regression model (1,2) if the condition (7) is locally satisfied, that is, if there exists a neighborhood Θ_θ of θ such that

$$\forall \theta' \in \Theta_\theta, \int_{\mathcal{X}} [\eta(x, \theta') - \eta(x, \theta)]^2 \xi(dx) = 0 \Rightarrow h(\theta') = h(\theta). \quad (24)$$

Consider again the case of a linear function of interest $h(\theta) = \mathbf{c}^\top \theta$ with the direction \mathbf{c} fixed. The next theorem indicates that when $\mathbf{c}^\top \theta$ is not (locally) estimable at θ^0 from the c -optimal design ξ^* it means that the support of ξ^* depends on the value θ^0 for which it is calculated. By combining different c -optimal designs obtained at various nominal values $\theta^{0,i}$ one can thus easily construct a nonsingular design from which θ , and thus $\mathbf{c}^\top \theta$, can be estimated. When the true value of $\bar{\theta}$ is not too far from the $\theta^{0,i}$'s, this design will be almost c -optimal for $\bar{\theta}$.

Theorem 4 *Consider a linear function of interest $h(\theta) = \mathbf{c}^\top \theta$, $\mathbf{c} \neq \mathbf{0}$, in a regression model (1,2) satisfying the assumptions $\mathbf{H1}_\eta$, $\mathbf{H2}_\eta$ and \mathbf{H}_h . Let $\xi^* = \xi^*(\theta^0)$ be a (local) c -optimal design minimizing $\mathbf{c}^\top \mathbf{M}^{-1}(\xi, \theta^0) \mathbf{c}$. Then, $h(\theta)$ being not locally estimable for ξ^* at θ^0 implies that the support of ξ^* varies with the choice of θ^0 .*

Proof. The proof is by contradiction. Suppose that the support of $\xi^*(\theta)$ does not depend on θ . We show that it implies that $h(\theta)$ is locally estimable at θ for ξ^* .

Suppose, without any loss of generality, that $\mathbf{c} = (c_1, \dots, c_p)^\top$ with $c_1 \neq 0$ and consider the reparametrization defined by $\beta = (\mathbf{c}^\top \theta, \theta_2, \dots, \theta_p)^\top$, so that $\theta = \theta(\beta) = \mathbf{J}\beta$ with \mathbf{J} the (jacobian) matrix

$$\mathbf{J} = \begin{pmatrix} 1/c_1 & -\mathbf{c}'^\top/c_1 \\ \mathbf{0}_{p-1} & \mathbf{I}_{p-1} \end{pmatrix},$$

where $\mathbf{c}' = (c_2, \dots, c_p)^\top$ and $\mathbf{0}_{p-1}, \mathbf{I}_{p-1}$ respectively denote the $(p-1)$ -dimensional null vector and identity matrix. From Elfving's Theorem,

$$\int_{\mathcal{S}^*} \frac{\partial \eta(x, \theta)}{\partial \theta} \xi^*(dx) - \int_{\mathcal{S}_{\xi^*} \setminus \mathcal{S}^*} \frac{\partial \eta(x, \theta)}{\partial \theta} \xi^*(dx) = \gamma \mathbf{c}$$

with $\gamma = \gamma(\theta) > 0$, \mathcal{S}_{ξ^*} the support of ξ^* and \mathcal{S}^* a subset of \mathcal{S}_{ξ^*} . Denote $\eta'(x, \beta) = \eta[x, \theta(\beta)]$. Since $\partial \eta'(x, \beta) / \partial \beta = \mathbf{J}^\top \partial \eta(x, \theta) / \partial \theta$ and $\mathbf{J}^\top \mathbf{c} = (1, \mathbf{0}_{p-1}^\top)^\top$, we obtain

$$\int_{\mathcal{S}^*} \frac{\partial \eta'(x, \beta)}{\partial \beta} \xi^*(dx) - \int_{\mathcal{S}_{\xi^*} \setminus \mathcal{S}^*} \frac{\partial \eta'(x, \beta)}{\partial \beta} \xi^*(dx) = \gamma[\theta(\beta)] \begin{pmatrix} 1 \\ \mathbf{0}_{p-1} \end{pmatrix}.$$

Therefore, $\int_{\mathcal{S}^*} \eta'(x, \beta) \xi^*(dx) - \int_{\mathcal{S}_{\xi^*} \setminus \mathcal{S}^*} \eta'(x, \beta) \xi^*(dx) = G(\beta_1)$, with $G(\beta_1)$ some function of β_1 , estimable for ξ^* . Finally, $\beta_1 = \mathbf{c}^\top \theta$ is locally estimable for ξ^* since $G(\beta_1)/d\beta_1 = \gamma[\theta(\beta)] > 0$. ■

Example (continued): Take $\mathbf{c} = (0, 1)^\top$, $\mathbf{c}^\top \theta$ is not locally estimable at $\theta^0 = (0.7, 0.2)^\top$ for the c -optimal design $\xi^* = \delta_{x_*}$, with $x_*(\theta^0) \simeq 4.28$, but the value of x_* depends on θ^0 through (20). Taking two different nominal values $\theta^{0,1}, \theta^{0,2}$ is enough to construct a nonsingular design by mixing the associated c -optimal designs. □

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