

Robust sequential designs for approximately linear models

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ABSTRACT

We consider the problem of the sequential choice of design points in an approximately linear model. It is assumed that the fitted linear model is only approximately correct, in that the true response function contains a nonrandom, unknown term orthogonal to the fitted response. We also assume that the parameters are estimated by M -estimation. The goal is to choose the next design point in such a way as to minimize the resulting integrated squared bias of the estimated response, to order n^{-1} . Explicit applications to analysis of variance and regression are given. In a simulation study the sequential designs compare favourably with some fixed-sample-size designs which are optimal for the true response to which the sequential designs must adapt.

RÉSUMÉ

Cet article porte sur la construction séquentielle de plans d'expérience dans le cadre de modèles approximativement linéaires. On part de l'hypothèse que le modèle linéaire dont les paramètres ont été déterminés par M -estimation est imparfait parce qu'il néglige un élément déterministe de la surface de réponse qui est orthogonal à la surface ajustée. On cherche alors à ajouter au plan expérimental le point pour lequel la réponse estimée ait le plus petit biais quadratique intégré possible, à l'ordre de $1/n$. On montre comment cette stratégie peut être mise en oeuvre en régression et en analyse de la variance. On montre aussi, à l'aide de simulations, que les plans séquentiels résultants soutiennent bien la comparaison avec certains plans à taille d'échantillon fixée, même quand ces derniers sont optimaux pour la courbe de réponse étudiée.

1. INTRODUCTION

In this paper we consider the problem of the sequential choice of design points in an approximately linear model.

Sequential designs for linear models have been studied by, among others, Fedorov (1972), Gebhardt and Heckendorff (1983) and Schwabe (1991). Schwabe (1990) establishes optimality properties of such designs in exactly linear models. The present work represents a departure from previously published work in simultaneously addressing the following points:

(1) It is assumed that the fitted linear model is only approximately correct. This introduces a bias into the estimates, which, to first order in n^{-1} , is minimized by the designs presented here. In some cases, in addition, estimates are provided of the nature

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of the inadequacy of the fitted model, thus guiding the experimenter in his choice of a more appropriate model.

(2) We assume that the parameters are estimated by (ordinary) M -estimation (see, e.g., Huber 1981). The combined design-estimation problem is thus robustified in two ways: against a misspecified response function, and against outlying observations.

In the remainder of this section, we make precise our notion of an “approximately linear” model, and give some examples. In Section 2 our approach to the sequential design problem is outlined in some generality. The case of M -estimated parameters is considered in Section 3. The examples are revisited in Section 4, where we propose some particular algorithms and demonstrate their properties.

We begin by supposing that the experimenter will take observations (\mathbf{x}_i, y_i) , where $\mathbf{x}_i : q \times 1$ is nonrandom but the y_i are observed with additive, i.i.d., zero-mean errors ε_i :

$$y_i := y(\mathbf{x}_i) = \mathcal{E}[y|\mathbf{x}_i] + \varepsilon_i, \quad \mathbf{x}_i \in S \subseteq \mathbb{R}^q.$$

The design space S may be a set over which \mathbf{x} varies freely, as in typical regression problems, or it may consist of a discrete set of coded levels, as in analysis-of-variance problems. We combine these and other cases by requiring the possible values of \mathbf{x} , and their relative importance, to be determined by a probability measure λ on S .

The experimenter chooses a vector of regressors $\mathbf{z}(\mathbf{x}) : p \times 1$ which, it is hoped, will adequately describe $\mathcal{E}[y|\mathbf{x}]$ in a linear manner, in that $\mathcal{E}[y|\mathbf{x}] \approx \boldsymbol{\theta}_*^T \mathbf{z}(\mathbf{x})$ for some $\boldsymbol{\theta}_*$ defined by $\boldsymbol{\theta}_* = \operatorname{argmin}_{\boldsymbol{\theta}} \int_S \{\mathcal{E}[y|\mathbf{x}] - \boldsymbol{\theta}^T \mathbf{z}(\mathbf{x})\}^2 d\lambda(\mathbf{x})$. Then with $f(\mathbf{x}) := \mathcal{E}[y|\mathbf{x}] - \boldsymbol{\theta}_*^T \mathbf{z}(\mathbf{x})$ it follows that

$$y(\mathbf{x}) = \boldsymbol{\theta}_*^T \mathbf{z}(\mathbf{x}) + f(\mathbf{x}) + \varepsilon, \quad (1.1)$$

$$\int_S f(\mathbf{x}) \mathbf{z}(\mathbf{x}) d\lambda(\mathbf{x}) = \mathbf{0}. \quad (1.2)$$

Note that $\boldsymbol{\theta}_*$ is uniquely defined by (1.1) and (1.2), as long as $\mathbf{A} := \int_S \mathbf{z}(\mathbf{x}) \mathbf{z}^T(\mathbf{x}) d\lambda(\mathbf{x})$ is nonsingular. This is assumed throughout.

Now suppose that n observations (\mathbf{x}_i, y_i) have been taken from the model described above. Define $N = n + 1$. We wish to determine a value $\mathbf{x}_N \in S$ at which to make the next observation on y . Our aim is to do this in such a way as to minimize, to order n^{-1} , the integrated (over S) squared bias (ISB) of the fitted values:

$$\begin{aligned} \text{ISB} &= \int_S \{\mathcal{E}[\hat{y}(\mathbf{x})] - \mathcal{E}[y|\mathbf{x}]\}^2 d\lambda(\mathbf{x}) \\ &= \mathcal{E}[\hat{\boldsymbol{\theta}}_N - \boldsymbol{\theta}_*]^T \mathbf{A} \mathcal{E}[\hat{\boldsymbol{\theta}}_N - \boldsymbol{\theta}_*] + \int_S f^2(\mathbf{x}) d\lambda(\mathbf{x}). \end{aligned}$$

Here, $\hat{y}(\mathbf{x}) = \hat{\boldsymbol{\theta}}_N^T \mathbf{z}(\mathbf{x})$. The estimate $\hat{\boldsymbol{\theta}}_N$ (an M -estimate) is defined precisely in Section 3 below. In Section 2, we will show that the optimal choice of \mathbf{x}_N is that which minimizes an inner product between the current value of the conditional bias $\hat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*$ and an empirical version of the influence function for $\hat{\boldsymbol{\theta}}_n$, evaluated at \mathbf{x} . These quantities are estimated by functionals of the residual process. The next observation is then to be made at the minimizer of the inner product of the estimates.

EXAMPLE 1.1. In the one-way layout, the fitted response is $\hat{y} = \sum_{j=1}^p \hat{\theta}_j x_j$, where x_j is the indicator of the event that the “treatment” is set at level j . The design space S may be

identified with the columns $\mathbf{z}_j = \mathbf{z}(\mathbf{x}_j)$ of the $p \times p$ identity matrix. Take $\lambda\{\mathbf{z}_j\} = p^{-1}$ for each j . Then (1.2) requires that f be identically zero on S , i.e., the fitted model is necessarily correct. However, the ISB arising from the M -estimation may still be reduced, relative to a fixed design, by a sequential allocation of treatments. A simple algorithm for determining such an allocation is given in Section 4.

EXAMPLE 1.2. Consider a 2^2 factorial experiment, with factors A and B each set at one of two levels, coded as ± 1 . The fitted response is $\hat{y}(\mathbf{x}) = \hat{\theta}_0 + \hat{\theta}_1 x_1 + \hat{\theta}_2 x_2$, with x_1 and x_2 denoting the levels of A and B respectively.

If the levels are quantitative, experimenters often add a centre point $(0, 0)$ to check for curvature. Then $S = \{(1, 1), (1, -1), (-1, 1), (-1, -1), (0, 0)\}$. Let λ be uniform on S . Then (1.2) is equivalent to

$$f(1, 1) = f(-1, -1) = \alpha, \quad f(1, -1) = f(-1, 1) = \beta, \quad f(0, 0) = -2(\alpha + \beta),$$

where α and β are arbitrary constants. This implies that on S ,

$$f(x_1, x_2) = \theta_3(x_1^2 + x_2^2 - 1.6) + \theta_4 x_1 x_2, \quad \theta_3, \theta_4 \text{ arbitrary,}$$

in which case

$$\mathcal{E}[y|\mathbf{x}] = \theta'_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3(x_1^2 + x_2^2) + \theta_4 x_1 x_2, \quad (1.3)$$

where $\theta'_0 = \theta_0 - 1.6\theta_3$. The enlarged model (1.3) is commonly fitted, when centre-point observations are available, in order to test the linearity of the response. See Montgomery (1984, Example 15.1).

EXAMPLE 1.3. If \mathbf{x} varies continuously over a design space S with positive Lebesgue measure, then (1.1) and (1.2) describe an approximately linear regression model. In Section 4 we will consider in particular the case of straight-line regression, for which $q = 1$ and $\mathbf{z}(x) = (1, x)^\top$. We take $S = [-\frac{1}{2}, \frac{1}{2}]$ and $\lambda = \text{Lebesgue measure}$. The model is then

$$y = \theta_0 + \theta_1 x + f(x) + \varepsilon, \quad \int_{-\frac{1}{2}}^{\frac{1}{2}} f(x) dx = \int_{-\frac{1}{2}}^{\frac{1}{2}} x f(x) dx = 0. \quad (1.4)$$

One fits a straight line to the data, but wishes the design to be robust against violations of linearity as represented by (1.4).

In this situation Huber (1975) obtained nonsequential designs, minimax with respect to squared error loss. Huber found the function f which maximized the risk [subject to an upper bound on $\int f^2(x) dx$] for a fixed design, and then the design which minimized this maximum risk. Wiens (1992) extended this approach to other fitted response functions and other loss functions. In both of these papers, the estimates were obtained by the method of least squares. Fixed designs combined with M -estimation are considered in Wiens (1994).

A feature of the approach we currently adopt is that, rather than *maximizing* the loss over f , we adaptively *estimate* f . A nonparametric estimate of the response function is computed from the first n observations. This allows for the estimation of the ISB; the N th observation is then made at a point \mathbf{x}_N chosen to maximize the decrease in the estimated ISB, to order n^{-1} . In the simulation study detailed in Section 4 the sequential designs compare favourably with some fixed-sample-size designs *which are optimal for the true response to which the sequential designs must adapt*.

2. SEQUENTIAL DESIGNS

Suppose that one has taken n observations (\mathbf{x}_i, y_i) from the model described in Section 1. Put $U_n = \{(\mathbf{x}_i, y_i) | i = 1, 2, \dots, n\}$, and compute an estimate $\hat{\boldsymbol{\theta}}_n = \boldsymbol{\theta}(U_n)$ of $\boldsymbol{\theta}_*$. Put $\hat{y}_n(\mathbf{x}) = \hat{\boldsymbol{\theta}}_n^\top \mathbf{z}(\mathbf{x})$. Now consider a sequence of such situations, and define, for $m \geq n$,

$$\text{ISB}(m|n) = \int_S \{\mathcal{E}[\hat{y}_m(\mathbf{x}) - \mathcal{E}[y|\mathbf{x}]|U_n]\}^2 d\lambda(\mathbf{x}),$$

the integrated squared bias, given U_n .

Given U_n , we seek to minimize the ISB resulting from one further observation, at a point $\mathbf{x}_N \in S$, with random error ε_N . (Recall that $N = n + 1$.) That is, we wish to make the next observation at $\mathbf{x}_N = \text{argmin}_{\mathbf{x}} \Delta(\mathbf{x}|U_n)$, where

$$\Delta(\mathbf{x}|U_n) = \text{ISB}(n+1|n) - \text{ISB}(n|n). \quad (2.1)$$

Note that the unconditional change in ISB is $\mathcal{E}_{U_n}[\Delta(\mathbf{x}|U_n)]$.

Writing $\|\mathbf{x}\|_A^2$ for $\mathbf{x}^\top \mathbf{A} \mathbf{x}$, we find

$$\int_S \{\mathcal{E}[\hat{y}(\mathbf{x}) - \mathcal{E}[y|\mathbf{x}]|U_n]\}^2 d\lambda(\mathbf{x}) = \|\mathcal{E}[\hat{\boldsymbol{\theta}}|U_n] - \boldsymbol{\theta}_*\|_A^2 + \int_S f^2(\mathbf{x}) d\lambda(\mathbf{x}). \quad (2.2)$$

In particular, since $\hat{\boldsymbol{\theta}}_n$ given U_n is nonrandom,

$$\text{ISB}(n|n) = \|\hat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*\|_A^2 + \int_S f^2(\mathbf{x}) d\lambda(\mathbf{x}). \quad (2.3)$$

Let H_n be the empirical distribution function of U_n , and consider estimators of the form $\hat{\boldsymbol{\theta}}_n = \boldsymbol{\theta}(H_n)$. Let $\delta_{\varepsilon, \mathbf{x}}$ denote the distribution function with all mass at $(\mathbf{x}, y(\mathbf{x})) = (\mathbf{x}, \mathcal{E}[y|\mathbf{x}] + \varepsilon)$. Then with $\eta := N^{-1}$, we have $H_N = (1 - \eta)H_n + \eta\delta_{\varepsilon, \mathbf{x}}$ for some $(\varepsilon, \mathbf{x})$, with \mathbf{x} to be determined. Define a function $b(\eta; \mathbf{x})$ by

$$b(\eta; \mathbf{x}) = \|\mathcal{E}[\boldsymbol{\theta}((1 - \eta)H_n + \eta\delta_{\varepsilon, \mathbf{x}})|U_n] - \boldsymbol{\theta}_*\|_A^2.$$

By (2.1)–(2.3),

$$\Delta(\mathbf{x}|U_n) = b(\eta; \mathbf{x}) - b(0; \mathbf{x}). \quad (2.4)$$

In order to apply Taylor's theorem to (2.4), we assume that b is twice differentiable on $[0, 1/n]$ with respect to η , and that $b'(\eta; \mathbf{x})$ may be obtained by differentiating under the integral sign.

With

$$\mathbf{d}_n(\varepsilon, \mathbf{x}; \eta) := \frac{d}{d\eta} \boldsymbol{\theta}((1 - \eta)H_n + \eta\delta_{\varepsilon, \mathbf{x}})$$

and $\mathbf{d}_n(\varepsilon, \mathbf{x}) := \mathbf{d}_n(\varepsilon, \mathbf{x}; 0)$, we calculate

$$b'(\eta; \mathbf{x}) = 2\{\mathcal{E}[\boldsymbol{\theta}((1 - \eta)H_n + \eta\delta_{\varepsilon, \mathbf{x}})|U_n] - \boldsymbol{\theta}_*\}^\top \mathbf{A} \mathcal{E}[\mathbf{d}_n(\varepsilon, \mathbf{x}; \eta)|U_n],$$

and hence

$$b'(0; \mathbf{x}) = 2(\hat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)^\top \mathbf{A} \mathcal{E}[\mathbf{d}_n(\varepsilon, \mathbf{x})|U_n].$$

Define

$$\tilde{\Delta}(\mathbf{x}|U_n) = \frac{b'(0; \mathbf{x})}{N} = \frac{2(\hat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)^\top \mathbf{A} \mathcal{E}[\mathbf{d}_n(\varepsilon, \mathbf{x})|U_n]}{N}. \quad (2.5)$$

By (2.4),

$$\Delta(\mathbf{x}|U_n) = \tilde{\Delta}(\mathbf{x}|U_n) + O_p(N^{-2}).$$

Given an estimate $\hat{\Delta}_n(\mathbf{x})$ of $\tilde{\Delta}(\mathbf{x}|U_n)$, we define

$$\hat{\mathbf{x}}_N = \operatorname{argmin}_{\mathbf{x}} \hat{\Delta}_n(\mathbf{x}).$$

Our prescription is then to take the next observation on y at $\mathbf{x} = \hat{\mathbf{x}}_N$.

REMARK 2.1. The term $\mathcal{E}[\mathbf{d}_n(\varepsilon, \mathbf{x})|U_n]$ may be viewed as a finite sample version of the influence function $\text{IF}(\mathbf{x})$ of $\hat{\boldsymbol{\theta}}_n$, and $\hat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*$ as the conditional value of the bias. In this sense, the point $\hat{\mathbf{x}}_N$ minimizes the inner product, with respect to the norm $\|\cdot\|_A$, between $\text{IF}(\mathbf{x})$ and the bias.

3. M -ESTIMATED PARAMETERS

Let $\psi(t)$ and $\chi(t)$ be respectively odd and even, bounded, absolutely continuous functions, weakly increasing for $t > 0$. Corresponding to Proposal 2 of Huber (1961, p. 96), we define $\hat{\boldsymbol{\theta}}_n$, and an auxiliary estimate $\hat{\sigma}_n$ of scale, to be roots of the $p + 1$ equations

$$\mathbf{0} = \frac{1}{n} \sum_{i=1}^n \boldsymbol{\Phi} \left(\mathbf{x}_i, \frac{y_i - \boldsymbol{\theta}_n^T \mathbf{z}(\mathbf{x}_i)}{\hat{\sigma}_n} \right), \quad (3.1)$$

where

$$\boldsymbol{\Phi}(\mathbf{x}, t) = \begin{pmatrix} \psi(t)\mathbf{z}(\mathbf{x}) \\ \chi(t) \end{pmatrix}.$$

Then $\boldsymbol{\theta}(H_N) = \boldsymbol{\theta}(\eta)$ and $\sigma(H_N) = \sigma(\eta)$ become functions of η via

$$\mathbf{0} = \int_S \boldsymbol{\Phi} \left(\mathbf{x}, \frac{y - \mathbf{z}^T(\mathbf{x})\boldsymbol{\theta}(\eta)}{\sigma(\eta)} \right) d\{(1 - \eta)H_n + \eta\delta_{\varepsilon, \mathbf{x}}\}. \quad (3.2)$$

In this notation, $\mathbf{d}_n(\varepsilon, \mathbf{x}) = \boldsymbol{\theta}'(0)$. We shall require as well $s_n(\varepsilon, \mathbf{x}) := \sigma'(0)$.

Differentiating (3.2) implicitly, we find

$$\begin{pmatrix} \mathbf{d}_n(\varepsilon, \mathbf{x}) \\ s_n(\varepsilon, \mathbf{x}) \end{pmatrix} = \mathbf{M}_n^{-1} \boldsymbol{\Phi}(\mathbf{x}, r_N(\varepsilon, \mathbf{x})),$$

where

$$\mathbf{M}_n = \frac{1}{\hat{\sigma}_n} \begin{pmatrix} \mathbf{T}_n & \mathbf{u}_n \\ \mathbf{v}_n^T & w_n \end{pmatrix},$$

$$\mathbf{T}_n = \frac{1}{n} \sum_{i=1}^n \psi'(r_i) \mathbf{z}(\mathbf{x}_i) \mathbf{z}^T(\mathbf{x}_i), \quad \mathbf{u}_n = \frac{1}{n} \sum_{i=1}^n r_i \psi'(r_i) \mathbf{z}(\mathbf{x}_i),$$

$$\mathbf{v}_n = \frac{1}{n} \sum_{i=1}^n \chi'(r_i) \mathbf{z}(\mathbf{x}_i), \quad w_n = \frac{1}{n} \sum_{i=1}^n r_i \chi'(r_i),$$

$$r_i = \frac{y_i - \mathbf{z}^T(\mathbf{x}_i) \hat{\boldsymbol{\theta}}_n}{\hat{\sigma}_n},$$

$$r_N(\varepsilon, \mathbf{x}) = \frac{\varepsilon + f(\mathbf{x}) - (\hat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)^T \mathbf{z}(\mathbf{x})}{\hat{\sigma}_n} = \frac{y_N(\mathbf{x}) - \hat{\boldsymbol{\theta}}_n^T \mathbf{z}(\mathbf{x})}{\hat{\sigma}_n}.$$

Thus

$$\mathbf{d}_n(\varepsilon, \mathbf{x}) = \mathbf{P}_n \mathbf{z}(\mathbf{x}) \psi(r_N(\varepsilon, \mathbf{x})) - \mathbf{q}_n \chi(r_N(\varepsilon, \mathbf{x})), \quad (3.3)$$

where

$$\mathbf{P}_n = \hat{\sigma}_n (\mathbf{w}_n \mathbf{T}_n - \mathbf{u}_n \mathbf{v}_n^\top)^{-1} \mathbf{w}_n, \quad \mathbf{q}_n = \hat{\sigma}_n (\mathbf{w}_n \mathbf{T}_n - \mathbf{u}_n \mathbf{v}_n^\top)^{-1} \mathbf{u}_n.$$

We will repeatedly use the fact that ε in $r_N(\varepsilon, \mathbf{x})$ is independent of U_n .

Define

$$\boldsymbol{\delta}_n = \int_S \mathcal{E} [\hat{\sigma}_n r_N(\varepsilon, \mathbf{x}) | U_n] \mathbf{z}(\mathbf{x}) d\lambda(\mathbf{x}). \quad (3.4)$$

A crucial observation is that then

$$\boldsymbol{\delta}_n = -\mathbf{A}(\hat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*).$$

From (2.5),

$$\tilde{\Delta}(\mathbf{x} | U_n) = -\frac{2\boldsymbol{\delta}_n^\top \mathcal{E} [\mathbf{d}_n(\varepsilon, \mathbf{x}) | U_n]}{N}. \quad (3.5)$$

We propose to substitute the (possibly smoothed) empirical residual process into the right-hand sides of (3.3) and (3.4), in order to construct estimates $\hat{\mathbf{d}}_n(\mathbf{x})$ and $\hat{\boldsymbol{\delta}}_n$ of $\mathcal{E} [\mathbf{d}_n(\varepsilon, \mathbf{x})]$ and $\boldsymbol{\delta}_n$. We then take the next observation at

$$\hat{\mathbf{x}}_N = \operatorname{argmax}_{\mathbf{x}} \hat{\boldsymbol{\delta}}_n^\top \hat{\mathbf{d}}_n(\mathbf{x}). \quad (3.6)$$

4. APPLICATIONS, EXAMPLES, MONTE CARLO

In this section we obtain explicit predictors $\hat{\boldsymbol{\delta}}_n$, $\hat{\mathbf{d}}_n(\mathbf{x})$ in several cases, and continue the examples of Section 1. We begin with the case of a finite design space.

4.1. Analysis of Variance.

Let the design space consist of M points $\{\mathbf{x}_1, \dots, \mathbf{x}_M\}$, and suppose that observations y_{ij} , $i = 1, \dots, n_j$, have been taken at \mathbf{x}_j . Define

$$r_{ij} = \frac{y_{ij} - \mathbf{z}^\top(\mathbf{x}_j) \hat{\boldsymbol{\theta}}_n}{\hat{\sigma}_n}, \quad \bar{r}_j = \sum_{i=1}^{n_j} r_{ij} / n_j, \quad (4.1)$$

$$l_j = \sum_{i=1}^{n_j} \psi(r_{ij}) / n_j, \quad m_j = \sum_{i=1}^{n_j} \chi(r_{ij}) / n_j,$$

$$\hat{\boldsymbol{\delta}}_n = \hat{\sigma}_n \sum_{j=1}^M \lambda\{\mathbf{x}_j\} \mathbf{z}(\mathbf{x}_j) \bar{r}_j, \quad (4.2)$$

$$\hat{\mathbf{d}}_n(\mathbf{x}_j) = \mathbf{P}_n \mathbf{z}(\mathbf{x}_j) l_j - \hat{\boldsymbol{\theta}}_n m_j. \quad (4.3)$$

The choice of the estimators in (4.2) and (4.3) is motivated in Remark 4.2 below.

REMARK 4.1. The estimate l_j at (4.1) is unsatisfactory if $M = p$ (as in the one-way layout), since then the definition of the M -estimator is precisely that each l_j vanishes. Also, from (1.2), $P_\lambda(f = 0) = 1$. In this case, we note that

$$\mathcal{E} [\psi(r_N(\varepsilon, \mathbf{x}_j)) | U_n] = \mathcal{E} \left[\psi \left(\frac{\varepsilon}{\hat{\sigma}_n} \right) \middle| U_n \right] + \mathcal{E} \left[\psi' \left(\frac{\varepsilon}{\hat{\sigma}_n} \right) \middle| U_n \right] \frac{(\boldsymbol{\theta}_* - \hat{\boldsymbol{\theta}}_n)^\top \mathbf{z}(\mathbf{x}_j)}{\hat{\sigma}_n} + \dots$$

The first term on the right vanishes asymptotically, and so we replace l_j by

$$l'_j = \frac{\bar{n}}{n} \bar{r}_j, \quad (4.4)$$

where $\bar{n} = \sum_{j=1}^p \sum_{i=1}^{n_j} \psi'(r_{ij})$.

EXAMPLE 1.1. (Continued). We have assumed ψ and χ to be bounded, so that the special case of least-squares estimation [$\psi(x) = x, \chi(x) = x^2 - 1$] is excluded. However, for the one-way layout, a *formal* evaluation of (3.5) for least squares gives

$$\bar{\Delta}(\mathbf{x}_j | U_n) = \frac{-2n\hat{\sigma}_n^2}{pN} \left| \frac{(\hat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)_j}{\sqrt{\bar{n}_j}} \right|^2, \quad (4.5)$$

so that we should aim to assign the next observation to that treatment for which the current value of $|(\hat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)_j|/\sqrt{\bar{n}_j}$ is a maximum. Schwabe (1990) derives this result for least squares under the condition $N \equiv 1 \pmod{p}$. He proposes replacing $\boldsymbol{\theta}_*$ by an initial guess, to apply the result.

A Monte Carlo study has indicated that for the M -estimators used, a direct application of (4.2) and (4.3) with the modification (4.4) leads to unsatisfactory designs. The algorithm tends to make very long strings of allocations to the same treatment group. The problem is that the dominant terms in $\hat{\Delta}_n$ arise from the last of the equations (3.1), and become nearly constant quite quickly as $\hat{\sigma}_n$ approaches its limiting value. If we ignore this equation, and treat the scale as fixed for the purpose of deriving $\mathbf{d}_n(\epsilon, \mathbf{x})$, then (4.3) and (4.4) give

$$\hat{\mathbf{d}}_n(\mathbf{x}_j) = \hat{\sigma}_n \mathbf{T}_n^{-1} \mathbf{z}_j l'_j = \frac{\bar{n} \hat{\sigma}_n \bar{r}_j}{\bar{n}_j} \mathbf{z}_j,$$

where $\bar{n}_j = \sum_{i=1}^{n_j} \psi'(r_{ij})$. Thus

$$\hat{\Delta}_n(\mathbf{x}_j) = \frac{-2\bar{n}\hat{\sigma}_n^2}{pN} \left| \frac{\bar{r}_j}{\sqrt{\bar{n}_j}} \right|^2,$$

directly analogous to (4.5). One should then assign the next observation to treatment j^* , where

$$j^* = \operatorname{argmax}_{1 \leq j \leq p} \frac{|\bar{r}_j|}{\sqrt{\bar{n}_j}}. \quad (4.6)$$

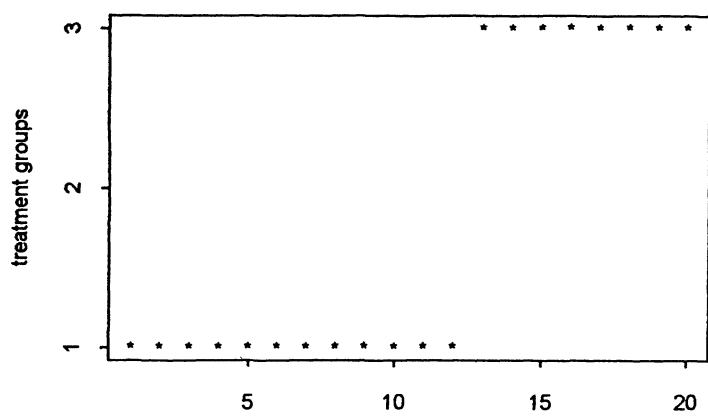
(This is, of course, not applicable to least squares, since then each $\bar{r}_j = 0$.)

Figure 1 shows a simulated sequence of designs determined by (4.6). There were $p = 3$ groups, with means $\theta_j = j$ and errors distributed according to a normal Student mixture:

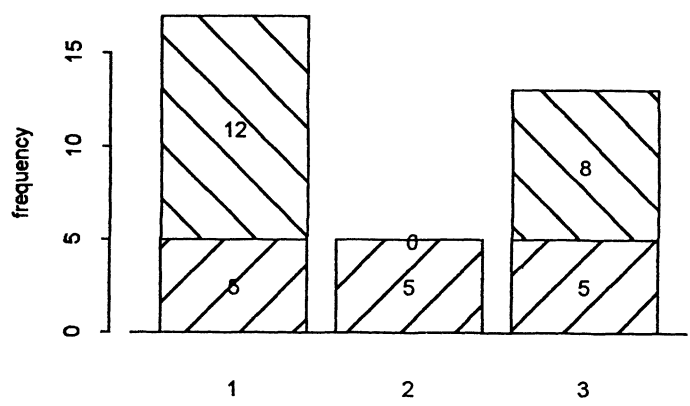
$$\varepsilon_{ij} \sim 0.8N(0, 1) + 0.2t_4.$$

We used Huber's $\psi(x) = \max(-k, \min(x, k))$ with [following a suggestion in Belsley, Kuh and Welsch (1980)] $k = 2\sqrt{p/n}$, and $\chi^2(x) = \psi^2(x) - \mathcal{E}_\Phi[\psi^2(X)]$. Note that then \bar{n}_j is the number of residuals with $|r_{ij}| < k$. The initial design had $n_1 = n_2 = n_3 = 5$ observations in each group.

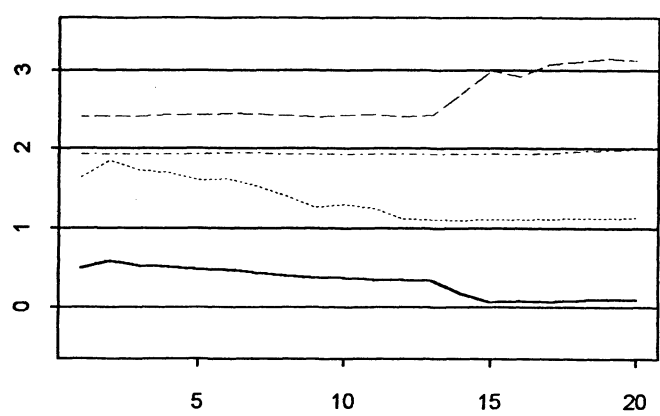
Figure 1(a) gives the sequence of points chosen via (4.6), 1(b) the current cumulative totals, and 1(c) the sequence of estimates, with horizontal lines at the target values θ_j , together with the values of $\{\sum(\hat{\theta}_j - \theta_j)^2/3\}^{1/2}$.



1a. Sequence of additional design points



1b. Initial and additional group frequencies



1c. Estimates (broken lines) and sample root-ISB (solid line)

FIGURE 1: One-way layout.

EXAMPLE 1.2. (Continued). Figure 2 shows a typical sequence of simulated 2^2 factorial designs with centre points. We applied (4.2) and (4.3) directly, with $\mathbf{z}(\mathbf{x}_j) = \mathbf{z}_j$ given by

$$\begin{aligned}\mathbf{z}_1^\top &= (1, 1, -1), & \mathbf{z}_2^\top &= (1, 1, 1), & \mathbf{z}_3^\top &= (1, 0, 0), \\ \mathbf{z}_4^\top &= (1, -1, 1), & \mathbf{z}_5^\top &= (1, -1, -1);\end{aligned}$$

with initially $n_1 = n_2 = n_4 = n_5 = 2$, $n_3 = 8$; and with $\lambda\{\mathbf{x}_j\} \equiv 0.2$. The true response is given by (1.3), with

$$\boldsymbol{\theta}_*^\top = (\theta_0, \theta_1, \theta_2) = (1, 2, 3), \quad \theta_3 = \theta_4 = \frac{5}{12}.$$

In Figure 2(c) the horizontal lines are at $\theta_0, \theta_1, \theta_2$ and at $\|f\| = (\int_S f^2 d\lambda)^{\frac{1}{2}} = 0.5$, the minimum attainable value of $(\text{ISB})^{\frac{1}{2}}$. The sample root-ISB is $\{\|f\|^2 + (\hat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)^\top \mathbf{A}(\hat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_*)\}^{\frac{1}{2}}$, where $\mathbf{A} = \text{diag}(1, 0.8, 0.8)$. The choices of ψ, χ and of the error distribution were as in Example 1.1.

The data give ample evidence of the inadequacy of the fitted model. We performed Wald's test of the hypothesis that $\theta_3 = \theta_4 = 0$ after choosing 0, 5 and 25 new points, obtaining p -values of 0.04, 0.0003 and 0.00008 respectively.

4.2. Regression.

Let $\hat{y}_n(\mathbf{x})$ be a nonparametric estimate of $\mathcal{E}[y(\mathbf{x})]$, computed from U_n . Define

$$\hat{r}_n(\mathbf{x}) = \frac{\hat{y}_n(\mathbf{x}) - \hat{\boldsymbol{\theta}}_n^\top \mathbf{z}(\mathbf{x})}{\hat{\sigma}_n}, \quad l(x) = \frac{1}{n} \sum_{i=1}^n \psi(r_i - \hat{r}_n(\mathbf{x}_i) + \hat{r}_n(\mathbf{x})),$$

$$m(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n \chi(r_i - \hat{r}_n(\mathbf{x}_i) + \hat{r}_n(\mathbf{x})),$$

$$\hat{\boldsymbol{\delta}}_n = \hat{\sigma}_n \int_S \hat{r}_n(\mathbf{x}) \mathbf{z}(\mathbf{x}) d\lambda(\mathbf{x}), \quad \hat{\mathbf{d}}_n(\mathbf{x}) = \mathbf{P}_n \mathbf{z}(\mathbf{x}) l(\mathbf{x}) - \hat{\boldsymbol{\theta}}_n m(\mathbf{x}).$$

As before, define $\hat{\mathbf{x}}_N$ by (3.5) and (3.6).

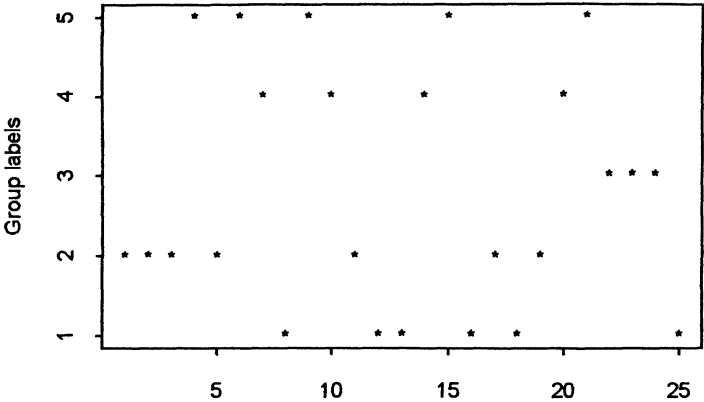
REMARK 4.2. The choice of the estimators is motivated as follows. Let $D_n(\mathbf{x}) = \hat{y}_n(\mathbf{x}) - \mathcal{E}[y(\mathbf{x})]$. Then

$$\hat{\boldsymbol{\delta}}_n - \boldsymbol{\delta}_n = \int_S D_n(\mathbf{x}) \mathbf{z}(\mathbf{x}) d\lambda(\mathbf{x})$$

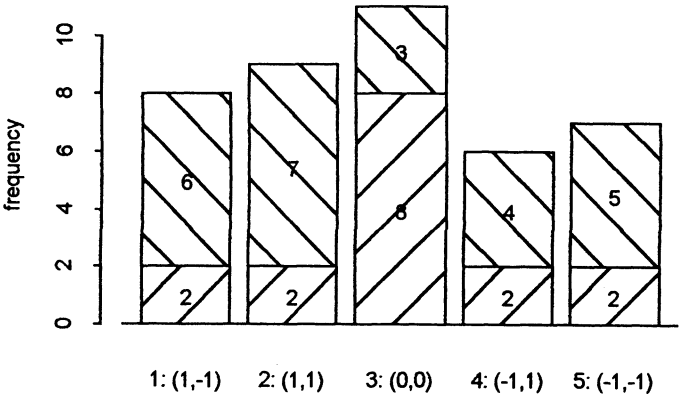
and

$$\begin{aligned}l(\mathbf{x}) - \mathcal{E}[\psi(r_N(\boldsymbol{\varepsilon}, \mathbf{x})) | U_n] \\ = \frac{1}{n} \sum_{i=1}^n \left\{ \psi \left(\frac{\varepsilon_i}{\hat{\sigma}_n} + \mathcal{E}[r_N(\boldsymbol{\varepsilon}, \mathbf{x})] \right) - \mathcal{E} \left[\psi \left(\frac{\varepsilon}{\hat{\sigma}_n} + \mathcal{E}[r_N(\boldsymbol{\varepsilon}, \mathbf{x})] \right) \right] \right\} + R_n,\end{aligned}$$

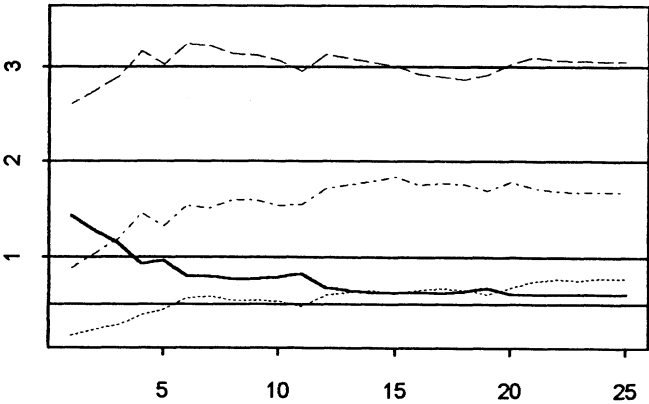
with a similar expression for $m(\mathbf{x})$, where the remainder R_n may be bounded by a multiple of $\sup_S |D_n(\mathbf{x})|$. Thus, if the smooth $\hat{y}_n(\mathbf{x})$ is consistent and the asymptotic dependencies among the ε_i are not too great, then $\hat{\boldsymbol{\delta}}_n, l$ and m will be consistent for



2a. Sequence of additional design points



2b. Initial and additional group frequencies



2c. Estimates (broken lines) and sample root-LSB (solid line)

FIGURE 2: Factorial design.

δ_n , $\mathcal{E} [\psi(r_N(\epsilon, \mathbf{x}))|U_n]$ and $\mathcal{E} [\chi(r_N(\epsilon, \mathbf{x}))|U_n]$ respectively. Similar considerations apply to (4.1)–(4.3).

EXAMPLE 1.3. (Continued). We have simulated sequences of designs for the model given by (1.4) with $\theta_0 = \theta_1 = 1$. The initial design consisted of 25 points: 6 each at $\pm \frac{1}{2}$, 3 each at $\pm \frac{3}{8}$, 2 each at $\pm \frac{1}{4}$, and 1 each at $\pm \frac{1}{8}$ and 0. The choices of ψ , χ and of the error distribution were as in the previous examples. We took $f(x)$ proportional to $x^2 - 12^{-1}$, normed so that $\|f\| = 0.25$. An estimate of f which is orthogonal to the regressors is given by

$$\hat{f}(x) = \hat{y}_n(x) - \mathbf{z}^T(x)\mathbf{A}^{-1} \int_S \mathbf{z}(x)\hat{y}_n(x) dx.$$

We used a Gaussian kernel smoother $\hat{y}_n(x)$, computed on S-PLUS, with a bandwidth varying from 0.5 to 0.3 as n increased. See Härdle (1990).

Figure 3(a) shows a plot of f , \hat{f} and the true and estimated regression lines after a further 60 observations have been taken. Figure 3(b) gives the sequence of design points. Figure 3(c) indicates that one should not expect to make substantial gains by taking more observations.

In Figure 3(d)–(f) the intercept estimates, slope estimates and sample root-ISBs [as in Example 1.2, with $\mathbf{A} = \text{diag}(1, \frac{1}{12})$] are plotted for the sequential designs as well as for several fixed-sample-size designs. In these plots the horizontal lines are at θ_0 [Figure 3(d)], at θ_1 [Figure 3(e)] and at $\|f\|$, the minimum attainable value of $(\text{ISB})^{\frac{1}{2}}$ [Figure 3(f)].

For each N from 26 to 85, each of the fixed-sample-size designs was constructed. Responses y_i were calculated using the same true mean response and the same random errors as for the sequential designs. M -estimates of the intercept, slope and scale parameters were then computed using the same ψ and χ as above.

The fixed-sample-size designs considered were:

(1) *Minimax*. This design was derived by Huber (1975). It minimizes the maximum integrated mean squared error of the fitted values, with the maximum taken over all f satisfying (1.4). The design has a density of the form $m_N(x) = a(1 + bx^2)^+$, with a and b depending on σ^2 and $\|f\|$. We used the *true* values $\sigma^2 = 1.2$, $\|f\| = 0.25$, and then computed design points $x_i = M_N^{-1}(i + 0.5/N)$, $i = 1, \dots, N$.

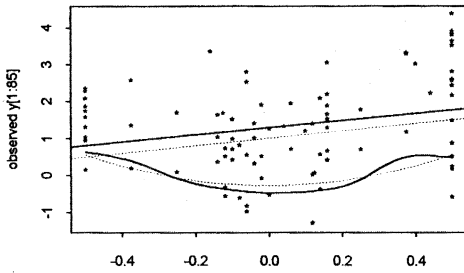
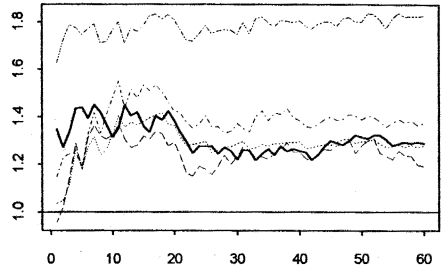
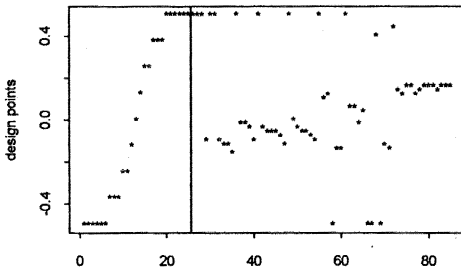
(2) *Maxpower*. For normal errors this design, with $\frac{1}{2}$ of the points at 0 and $\frac{1}{4}$ at each of $\pm \frac{1}{2}$, is most powerful for distinguishing a quadratic response from a straight line. See Huber (1975, p. 294).

(3) *Minbias*. This design minimizes the ISB of the fitted values when a straight line is fitted to a quadratic mean response. It places $\frac{2}{3}$ of the observations at 0, and $\frac{1}{6}$ at each of $\pm \frac{1}{2}$.

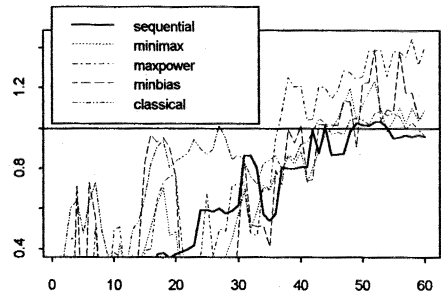
(4) *Classical*. This is the optimal design if the mean response is exactly linear. There are $[N/2]$ points at each of $\pm \frac{1}{2}$, with 1 point at 0 if N is odd.

As expected, the classical designs performed very poorly with respect to estimation of the intercept. Because of the symmetry of the contamination, the slope was accurately estimated. The sequential designs outperformed the maxpower designs, and performed as well overall as the minimax and minbias designs, despite being required to adapt to the form of the alternative response (or the parameters, in the minimax case) for which these other designs are optimal.

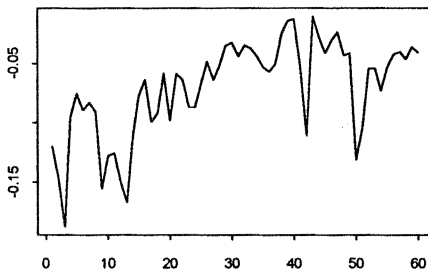
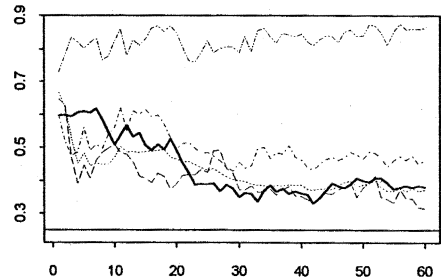
Our general conclusion is that a sequential strategy as adopted here can produce

3a. $f(x)$ and reg'n line: est'd (solid) and true (dotted)3d. Intercept estimates vs. (N-25) for various sequences of designs
Legend is with Fig. 3e

3b. Original design, with additional points chosen sequentially



3e. Slope estimates vs. (N-25) for various sequences of designs

3c. Minima of $N\hat{\Delta}$ vs. (N-25)3f. Sample root-1SB vs. (N-25) for various sequences of designs
Legend is with Fig. 3eFIGURE 3: Straight-line regression (true response is quadratic), $N = 85$.

significant gains in the presence of unspecified contamination of the response function and/or error distribution.

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