The Annals of Statistics
1984, Vol. 12, No. 4, 1324–1348

SOME MODEL ROBUST DESIGNS IN REGRESSION

BY JEROME SACKS[1] AND DONALD YLVISAKER[2]

Northwestern University and University of California, Los Angeles

We dedicate this paper to the memory of
Jack Kiefer—teacher, colleague, and, above all, friend.

Theory for finding designs in estimating a linear functional of a regression function is developed for classes of regression functions which are infinite dimensional. These classes can be viewed as representing possible departures from an "ideal" simple model and thus describe a model robust setting. The estimates are restricted to be linear and the design (and estimate) sought is minimax for mean square error. The structure of the design is obtained in a variety of cases; some asymptotic theory is given when the functionals are integrals. As to be expected, optimal designs depend critically on the particular functional to be estimated. The associated estimate is generally not a least squares estimate but we note some examples where a least squares estimate, in conjunction with a good design, is adequate.

0. Introduction. Let T be a set of sites. An observation at $t \in T$ is assumed to be of the form

$$Y_t = f(t) + \sigma \cdot \varepsilon_t \tag{0.0}$$

where $E\varepsilon_t = 0$, $E\varepsilon_t^2 = 1$ and $f \in \mathscr{F}$, a class of possible regressions over T. This paper fixes certain $\mathscr{F}$'s (see (0.4)) and deals with designs, that is, placement of uncorrelated observations in T, for the estimation of regression parameters.

The class $\mathscr{F}$ can be one of the standard classes, such as polynomials of fixed degree, but our intent is to treat problems where $\mathscr{F}$ is not finite dimensional and thereby develop some theory about designs which are robust against departures of f from a standard simple model and, more generally, to treat designs for estimating characteristics of a nonparametric regression function. For example, suppose $T = [-1, 1]$ and $\mathscr{F}$ is a class of functions on T with bounded second derivative, namely, $\{f \mid |f''(t)| \le M, \text{ all } t\}$ where M is specified. This $\mathscr{F}$ can be thought of as a class of nearly linear functions (it clearly includes all linear functions) and serves to represent departure from the "ideal" model where f is linear. Generally, we envision problems where a precise (finite dimensional) model cannot be safely specified but where certain linear functionals of the regression function, which we call parameters, are of special interest. In the above example we might be interested in the estimation of $f(0)$ or $f(1) - f(-1)$

Received October 1982; revised April 30, 1984.

[1] This author's work was supported in part by NSF Grant #MCS-81-18582.

[2] This author's work was supported in part by NSF Grant #MCS-80-02732.

AMS 1980 subject classifications. Primary 62K05; secondary 62J02.

Key words and phrases. Optimal design, model robustness, regression design, approximately linear models, nonparametric regression, linear estimation, minimax designs.

or $\int_0^1 f(t)\,dt$. The question we address is: how do we design the observations to accomplish the estimation in an optimal way?

The specification of $\mathscr{F}$ is an approximation for the "real" f whose explicit form can never be known. Thus the choice of a finite dimensional polynomial class gives a specific approximation and an estimate of a coefficient of the polynomial is an estimate of a linear functional of the *approximation* rather than a characteristic of f itself. It is a consequence of the finite dimensionality that there is then ambiguity about what characteristic of f is being estimated. For example, if f is in the class of straight lines on $[-2, 2]$ then there is no difference between the linear functionals $(f(1) - f(-1))/2$ and $f'(0)$. However, if f is viewed as a member of a larger class, for example, $\mathscr{F}_2 = \{f \mid |f''(x)| \le M\}$, then the two linear functionals on $\mathscr{F}_2$ are distinct. The effect on designs will be seen to be considerable: within the smaller model a best design for either functional is to put half the observations at -2 and half at $+2$ while in the larger model the best designs are markedly different, the first functional requiring placement of observations nearer to -1 and $+1$ while the second functional requires observations nearer to 0 (see Examples, 2.1 and 3.1).

The original work introducing concern about departures from a "parsimonious" model is by Box and Draper (1959) who investigate the design consequences of using the smaller model for estimation in a larger but finite dimensional class; thus, the smaller model may be the linear functions while the larger class consists of quadratics. The subsequent interesting papers of Karson, Manson and Hader (1969), Kiefer (1973, 1980), Draper and Herzberg (1976) and Galil and Kiefer (1977) also resort to finite dimensional classes and, necessarily, retain the ambiguity about what properties of f are being estimated.

A reflection of the confusion caused by this ambiguity is the widely held view that, in the traditional fitting of a straight line, the optimal design, which divides the observations equally among the two most extreme available sites, is objectionable because it requires specifying the extreme sites and because it provides no information at intermediate points in order to assess the validity of a straight line fit. It is our view that clear objectives stated in terms of characteristics of the underlying f can provide a rationale for choices of design which deals with the type of objections described above and does not suffer from ambiguities caused by appealing first to an approximation of f.

We concentrate here on treating specific linear functions of f; we do not address the curve fitting problem. Huber's (1975) formulation of curve fitting is a step towards providing a more relevant model, albeit a halting one since no implementable design can serve in that formulation; another approach to curve fitting is taken by Agarwal and Studden (1978).

The pertinent and more exacting task of exploring problems involving several functionals simultaneously is deferred; such a study for a specific pair of functionals $(f(0), f'(0))$ was initiated in Marcus and Sacks (1976) for an infinite dimensional model slightly different than the ones we consider in this paper and related studies were carried out by Li and Notz (1982), Pesotchinsky (1982) and Li (1984).

Our attention is limited to estimates which are linear functions of the observations. When $\mathscr{F}$ is a finite-dimensional vector space (e.g., all polynomials of fixed degree) and the ε's are normal this is no restriction if a minimax approach is adopted since least squares is minimax for squared error loss.

However, when $\mathscr{F}$ is an infinite dimensional class (like those in (0.4)) which can be thought of as representing the departures from an "ideal" simpler linear model there is, necessarily, a bias term which is introduced and it is generally true that the least squares estimates connected with the ideal model will not suffice for minimaxing mean square error even among linear estimates (Example 1.2). A similar observation was at the heart of the treatment by Karson, Manson, Hader (1969). Various authors cited earlier assume the use of least squares estimation based on the parsimonious model (e.g., Box and Draper, 1959; Huber, 1975; Agarwal and Studden, 1978; Pesotchinsky, 1982) although it is by no means certain that the optimal choice of both design and linear estimates leads to least squares nor is there much a priori justification for adherence to least squares. In some examples least squares can be optimal (see Marcus and Sacks, 1976; Li and Notz, 1982); and in other examples, the marriage of the least squares estimate with a good design may serve to provide adequate suboptimal solutions (see Sections 4 and 5, and Marcus and Sacks, 1976), but the general utility of least squares remains an open issue.

The restriction to linear estimates rules out the possiblity of considering gross errors in the distribution of the ε's even for finite dimensional $\mathscr{F}$. When $\mathscr{F}$ is more general, for example the class of functions with bounded derivative, we may be interested in functionals which are bounded, such as $f(1) - f(-1)$. In such a case linear estimates cannot be optimal, and if the bound is small enough, and the observations are few enough, there is evidence that substantial improvement may be available (Cassella and Strawderman, 1981). At the very least, truncation of the linear estimates would be preferred. Fortunately, the effect of the boundedness is likely to be minimal for reasonably sized n and we do not regard this aspect as a serious failure of linear estimates.

Even when the parameter is unbounded the minimax linear estimate is not minimax among all estimates in the models of (0.4) (Sacks and Strawderman, 1982). Moreover, it is shown there that the minimax linear estimates are typically *not* asymptotically minimax as the sample size goes to ∞ unless the observations accumulate rapidly at a few sites. The designs for the parameters in Sections 1 and 2 have this property so that we do not regard the use of linear estimates in those contexts as potentially troublesome at least for reasonable n. In the context of Sections 4 and 5, where the designs are more diffuse, asymptotic minimaxity of linear estimates will not hold; nonetheless, the gain achievable by use of alternate estimates may not be substantial and, in any case, the designs suggested appear to be reasonable ones.

Mathematical Preliminaries. Our mathematical development begins with a space $\mathscr{F}$ of functions on T, a linear functional Γ defined on $\mathscr{F}$ and n uncorrelated observations satisfying (0.0). Suppose the n observations are such that $n_i \geq 1$ are located at sites t_i, $i = 1, \cdots, k$. The design problem we pose is to choose k, $\mathbf{n} = (n_1, \cdots, n_k)$, $\mathbf{t} = (t_1, \cdots, t_k)$ and $\mathbf{c} = (c_1, \cdots, c_k)$ to minimize

$$J(k, \mathbf{n}, \mathbf{t}, \mathbf{c}) = \sup_{\mathscr{F}} E_f(\textstyle\sum_{i=1}^k c_i \bar{Y}_{t_i} - \Gamma f)^2 \tag{0.1}$$
$$= \sigma^2 \textstyle\sum_{i=1}^k (c_i^2/n_i) + \sup_{\mathscr{F}}(Cf - \Gamma f)^2$$

where C is the linear functional defined by

$$Cf = E_f(\textstyle\sum_{i=1}^k c_i \bar{Y}_{t_i}) = \sum_{i=1}^k c_i f(t_i) = \displaystyle\int_T f\, dC.$$

(Here the functional C is identified with the measure it induces. We shall also use the notation $C(x)$ to denote the value of the induced distribution function at x.) The minimization of (0.1) is called the *exact* problem. If J is optimized with respect to $\mathbf{n}$ for fixed k, $\mathbf{t}$, $\mathbf{c}$ and without regard to the integer nature of the n_i's, the resulting minimum occurs when $n_i/n_k = |c_i|/|c_k|$, $i = 1, \cdots, k$, and has value

$$J(k, \mathbf{t}, \mathbf{c}) = (\sigma^2/n)(\textstyle\sum_{i=1}^k |c_i|)^2 + \sup_{\mathscr{F}}(Cf - \Gamma f)^2. \tag{0.2}$$

The minimization, of (0.2) by choice of k, $\mathbf{t}$, $\mathbf{c}$ (equivalently by choice of C) is called the *approximate* problem. If C^* is optimum for (0.2) and $\mathbf{n}^*$ has noninteger values, then implementation of the design requires replacement of the n_i^* by integers. When C^* calls for many sites (relative to n) the implementation is troublesome; otherwise the comparative tractability of (0.2) to (0.1) makes the approximate approach advantageous.

If $\mathscr{F}$ is a finite dimensional linear space, say $\{f \mid f = \sum_{i=1}^d \alpha_i f_i$ for some $\alpha_1, \cdots, \alpha_d\}$, then Γ is a linear combination of the regression coefficients $\{\alpha_i\}$ and, with k, $\mathbf{n}$ and $\mathbf{t}$ fixed, (0.1) calls for the minimax mean square error estimation of Γ. The supremum over $\mathscr{F}$ of the mean square error will be finite only when an unbiased estimate is used, so one is led to the least squares estimation of Γ. The subsequent minimization with respect to $\mathbf{n}$ and $\mathbf{t}$ is a central problem in standard design theory and has been extensively studied (Guest, 1958; Hoel, 1958; Kiefer and Wolfowitz, 1959; Kiefer, 1961; Karlin and Studden, 1966; Wynn, 1970; Fedorov, 1972, are important early papers).

The functionals Γ we will treat for infinite dimensional $\mathscr{F}$ are

(0.3)
i) Discrete: $\Gamma f = \sum_{j=1}^N \gamma_j f(x_j) = \int f\, d\Gamma$,

ii) Continuous: $\Gamma f = \int \gamma(x) f(x)\, dx$,

iii) Derivatives (when appropriate): $\Gamma f = f'(x_0)$.

In the finite dimensional settings we discuss (see (0.4)), these parameters (functionals) are uniquely determined, in contrast with the finite dimensional set-up where, for example, if $\mathscr{F} = \{\alpha + \beta x$, some $\alpha, \beta\}$ on $[-1, 1]$, then α and β have representations as

$$\alpha = f(0) = \frac{f(1) + f(-1)}{2} = \frac{1}{2} \int_{-1}^{1} f(x)\, dx,$$

$$\beta = f'(0) = \frac{f(1) - f(-1)}{2} = \frac{3}{2} \int_{-1}^{1} x f(x)\, dx$$

among others.

Here are the $\mathscr{F}$'s we consider. With $T = R^1$

$$(0.4)\quad \begin{aligned} \mathscr{F}_1 &= \mathscr{F}_1(M) = \{f \mid |f(x) - f(y)| \le M|x - y|, \text{ for every } x, y \in T\} \\ &\supset \mathscr{F}_1^0(M) = \{f \mid |f'(x)| \le M, \text{ all } x\} \supset \{\text{constants}\}. \\ \mathscr{F}_2 &= \mathscr{F}_2(M) = \{f \mid f' \in \mathscr{F}_1(M)\} \\ &\supset \mathscr{F}_2^0(M) = \{f \mid f' \in \mathscr{F}_1^0(M)\} \supset \{\text{linear functions}\}. \end{aligned}$$

The restriction to R^1 is a substantial one; we hope to address multidimensional T at another time. In order to avoid added complications, we do not consider subsets T of R^1 but results about such problems can be obtained by following the arguments we present.

The placement of f in $\mathscr{F}_1$ or $\mathscr{F}_2$ is an assumption about its smoothness $-f$ or its derivative satisfies a uniform Lipschitz condition. It turns out that the theory appropriate for $\mathscr{F}_1$ or $\mathscr{F}_2$ is the same as that for $\mathscr{F}_1^0$ or $\mathscr{F}_2^0$, respectively, so one can begin with either type of condition about f. Since $\mathscr{F}_1$ contains constant functions—indeed the constants represent the intersection of the classes $\mathscr{F}_1(M)$ over $M > 0$—it can be viewed as a collection of nearly constant regressions. Similarly, since $\mathscr{F}_2$ contains all linear functions it can be taken to be a model for nearly linear regressions. Huber (1975) has solved the problem of design for extrapolation from a half-line in the $\mathscr{F}_k^b(M)$ setting.

There are, of course, other $\mathscr{F}$'s of interest. The choice here is motivated by some knowledge of minimax linear estimation for these spaces (Sacks and Ylvisaker, 1978), their general acceptability and their (relative) simplicity. Dei-in Tang is investigating Sobolev spaces, in response to the work on estimation that has been done there (Speckman, 1979). Spruill (1982) has recently treated some general questions on extrapolation when $\mathscr{F}$ is a Sobolev space.

The paper is organized in a straightforward way. Successive sections will deal with discrete parameters, nonsmooth ($\mathscr{F}_1$) and smooth ($\mathscr{F}_2$) cases; derivatives in $\mathscr{F}_2$; continuous parameters, nonsmooth and smooth cases. One reason to set matters up in this way is to attempt a contrast of results according to the degree of smoothness which is assumed. Each section contains relevant theory, several examples, and some efficiency calculations for the obtained estimates and designs when they are employed in standard models. The final sections on continuous parameters contain some asymptotic theory—we allow $n \to \infty$ for fixed σ^2 and M. There is the customary interplay between these three parameters and one important aspect of the relationship is carried by the parameter $\rho = nM^2/\sigma^2$, as can be seen at (0.2). Some reduction in complexity occurs if one adopts an error-scaled model—take $M = \sigma\tilde{M}$ and get $\rho = n\tilde{M}^2$.

The choice of M, σ^2 (or $\tilde{M}$) is clearly relevant. For design problems we cannot ask that the data inform us about proper choices via crossvalidation, for example. It is relevant therefore to evaluate the qualities of a design for different plausible values of M, σ^2 as indicated in some of the examples we present.

1. $\mathscr{F}_1$, Discrete parameters. We use the notation set at (0.3) and (0.4) where the parameter Γ is identified with a discrete signed measure whose support we denote by $S(\Gamma)$. By C^* we mean an optimum functional (if it exists) associated with (0.1) or (0.2) depending on the context, and $S(C^*)$ denotes its support. We shall, in fact, show the basic result for both the exact and approximate problems, that the support of the optimum design can be sharply limited and that an optimum C^* exists (Proposition 1.1). In Proposition 1.2 we show that the approximate problem has $C^* = \Gamma$ if Γ is a positive functional. Later propositions provide some structure for C^* which we use to calculate a number of examples exhibiting various behavior.

The space $\mathscr{F}_1$ contains all constants and a functional C cannot correspond to the minimum at (0.1) or (0.2) unless $C1 = \Gamma 1$. For a C with finite support write

$$Cf - \Gamma f = \sum_{i=1}^{k} c_i f(t_i) - \sum_{j=1}^{N} \gamma_j f(x_j) = \sum_{i=1}^{m} a_i f(z_i)$$

with $z_1 < \cdots < z_m$ and $\sum_{i=1}^{m} a_i = 0$. Thus $\{z_1, \cdots, z_m\} = S(C) \cup S(\Gamma)$. Now

$$|Cf - \Gamma f| = |\sum_{i=1}^{m} a_i f(z_i)| = |\sum_{i=2}^{m} A_i(f(z_i) - f(z_{i-1}))| \le M \sum_{i=2}^{m} |A_i| |A_i| \delta_i$$

for all $f \in \mathscr{F}_1$ where $A_i = \sum_{j=i}^{m} a_i$ and $\delta_i = z_i - z_{i-1}$, $i = 2, \cdots, m$. Moreover, equality is achieved when $f(z_i) - f(z_{i-1}) = M\delta_i \operatorname{sgn} A_i$, $i = 2, \cdots, m$. Thus (0.1) becomes

$$J(k, \mathbf{n}, \mathbf{t}, \mathbf{c}) = \sigma^2 \sum_{i=1}^{k} (c_i^2/n_i) + M^2(\sum_{i=2}^{m} |A_i| \delta_i)^2, \tag{1.1}$$

and (0.2) can be written as

$$J(C) = \frac{\sigma^2}{n} (\sum_{i=1}^{k} |c_i|)^2 + M^2(\sum_{i=2}^{m} |A_i| \delta_i)^2. \tag{1.2}$$

Observe here that, while the definition of J in (1.2) could be extended, the domain of J is taken to be finitely supported C's and we minimize accordingly.

PROPOSITION 1.1. *For* (1.1) *or* (1.2) *there is an optimum* C^* *with* $S(C^*) \subset S(\Gamma)$.

PROOF. Begin with (1.1) and suppose that $C1 = \Gamma 1$. If there are elements $z_s < z_{q+1}$ in $S(\Gamma)$ with $z_{s+1}, \cdots, z_q$ in $S(C) - S(\Gamma)$ and if

$$|A_r| = \min(|A_{s+1}|, \cdots, |A_{q+1}|),$$

move the observations at $z_r, \cdots, z_q$ to z_{q+1}, those at $z_{s+1}, \cdots, z_{r-1}$ to z_s and replace Cf by $\tilde{C}f = \sum_{i=1}^{s} c_i f(t_i) + f(t_s) \sum_{s+1}^{n-1} c_i + f(t_{q+1}) \sum_{r}^{q} c_i + \sum_{q+1}^{k} c_i f(t_i)$. The variance term in (1.1) is not increased by this change while the bias term,

$\sum_{s+1}^{q+1} |A_i| \delta_i$, gets replaced by $(\sum_{s+1}^{q+1} \delta_i) |A_r|$ which is also not an increase ($|A_s|$ remains the same as do all the other A's). If, say, $z_{q+1} = x_1$, then move the observations left of x_1 to x_2 itself and find J to be no larger. Thus we may restrict attention to C's with support contained in $S(\Gamma)$. For fixed $\mathbf{n}$ the minimum of (1.1) is achieved at some $\mathbf{c}$ since J is continuous in $\mathbf{c}$ and goes to ∞ as $|\mathbf{c}| \to \infty$. Subsequent minimization over $\mathbf{n}$ shows that, in the exact case, an optimum must exist. The approximate case is argued in the same way.

We turn next to finding the solution to the approximation problem (1.2). In view of Proposition 1.1, take $z_i = x_i$ for $i = 1, \cdots, N$, with $c_j = 0$ if x_j is not a point in the support of C. Standard notation is used in writing $\Gamma = \Gamma^+ - \Gamma^-$ to indicate the decomposition of a signed measure into its positive and negative parts.

PROPOSITION 1.2. *If Γ is a positive measure or a negative measure then $C^* = \Gamma$ is the unique solution to* (1.2). *Otherwise, Γ is not optimum.*

PROOF. If $C1 = \Gamma 1$ and Γ is a positive measure, then

$$J(C) \geq \frac{\sigma^2}{n} (\textstyle\sum_{j=1}^N |c_j|)^2 \geq \frac{\sigma^2}{n} (\sum_{j=1}^N c_j)^2 = \frac{\sigma^2}{n} (\sum_{j=1}^N \gamma_j)^2 = J(\Gamma)$$

and the first inequality is strict unless $C = \Gamma$. On the other hand if $\Gamma = \Gamma^+ - \Gamma^-$ with $\Gamma^+(1)\Gamma^-(1) > 0$ it is not hard to show that Γ is worse than $C_\varepsilon = (1 - \varepsilon)\Gamma^+ - (1 - \varepsilon(\Gamma^+(1)/\Gamma^-(1)))\Gamma^-$ for small positive ε.

From now on Γ will be an honest signed measure as we try to minimize J. For perturbing a given C we use the notation $\tilde{C} = \tilde{C}_{i,j}$ where $\tilde{c}_i = c_i - \varepsilon$, $\tilde{c}_j = c_j + \varepsilon$, $\tilde{c}_q = c_q$ otherwise.

PROPOSITION 1.3. *If C^* is optimum for* (1.2), *$C^{*+} \leq \Gamma^+$ and $C^{*-} \leq \Gamma^-$.*

PROOF. Suppose $c_i > 0$ and $c_i > \gamma_i$, for some $2 \leq i \leq N - 1$. From the definition of A_i (see (1.1) above) $A_i = A_{i+1} + c_i - \gamma_i$. If C is changed to $\tilde{C} = \tilde{C}_{i,i-1}$ then $\tilde{A}_i = A_i - \varepsilon$ and $\tilde{A}_q = A_q$ if $q \neq i$. Therefore, if $A_i > 0$ and ε is small $\sum |A_j| \delta_j > \sum |\tilde{A}_j| \delta_j$ and $\sum |c_j| \geq \sum |\tilde{c}_j|$ so $J(\tilde{C}) < J(C)$. If $A_i \leq 0$ then $A_{i+1} = A_i - c_i + \gamma_i < 0$. Now use $\tilde{C} = \tilde{C}_{i,i+1}$ and get $\tilde{A}_{i+1} = A_i - c_i + \gamma_i + \varepsilon = A_{i+1} + \varepsilon$ so $|\tilde{A}_{i+1}| < |A_{i+1}|$ if ε is small enough. Since $\tilde{A}_q = A_q$ for $q \neq i + 1$, $\sum |A_j| \delta_j > \sum |\tilde{A}_j| \delta_j$ and $\sum |c_j| \geq \sum |\tilde{c}_j|$, implying $J(\tilde{C}) < J(C)$.

If $i = N$ then $A_N = c_N - \gamma_N > 0$ and the first part of the proof using $\tilde{C} = \tilde{C}_{N,N-1}$ shows that $J(\tilde{C}) < J(C)$. If $i = 1$ then $A_2 = A_1 - c_1 + \gamma_1 = -c_1 + \gamma_1 < 0$ and we use the second part of the proof with $\tilde{C} = \tilde{C}_{1,2}$ to get $J(\tilde{C}) < J(C)$.

PROPOSITION 1.4. *If n is sufficiently large and C^* is optimum for* (1.2) *with $S(C^*) \subset S(\Gamma)$ then*

(i) $S(C^*) = S(\Gamma)$,
(ii) $\gamma_j \gamma_{j-1} > 0$ *implies* $A_j^* = 0$,
(iii) $\gamma_j > 0$ *implies* $A_j^* \leq 0$, $\gamma_j < 0$ *implies* $A_j^* \geq 0$.

Proof. The minimum value of (1.2) is $O(1/n)$ since

$$J(\Gamma) = (\sigma^2/n)(\sum_{j=1}^N |\gamma_j|)^2.$$

Therefore, for an optimum C^*, $|A_i^*| = O(1/\sqrt{n})$ for $i \geq 2$, and then,

$$|c_i^* - \gamma_i| = |A_i^* - A_{i+1}^*| = O(1/\sqrt{n}) \text{ for } i \geq 1.$$

This guarantees that, for sufficiently large n, every c_i^* differs from zero, thereby establishing (i).

From (i) we have $c_j^* \neq 0$ for all j. If $\sum_2^N |A_j^*| \delta_j = 0$ then all $A_j^* = 0$ (and $c_j^* = \gamma_j$) and there is nothing to prove. Otherwise, let

$$\rho = nM^2/\sigma^2,\ \lambda_1 = \sum_1^N |c_j^*|,\ \lambda_2 = \rho \sum_2^N |A_j^*| \delta_j$$

and then $\lambda_1, \lambda_2 > 0$. Recall that $c_j = \gamma_j + A_j - A_{j+1}(A_1 = A_{N+1} = 0)$ and define

$$K(A) = (\sum_1^N |\gamma_j + A_j - A_{j+1}|)^2 + \rho(\sum_2^N |A_j| \delta_j)^2.$$

Since K is minimized at A^* let η_j be the unit vector with 1 in the jth position, $j = 2, \cdots, N$ and calculate, if $A_j^* \neq 0$,

$$\begin{aligned} 0 &\leq \tfrac{1}{2} [K(A^* + h\eta_j) - K(A^*)] \\ &= \lambda_1 h \operatorname{sgn}(c_j^*) - \lambda_1 h \operatorname{sgn}(c_{j-1}^*) + \lambda_2 h \operatorname{sgn}(A_j^*)\delta_j + O(h^2). \end{aligned}$$

Letting $h \downarrow 0$ and $h \uparrow 0$ produces, for $j = 2, \cdots, N$,

$$\lambda_2 \operatorname{sgn}(A_j^*)\delta_j = \lambda_1[\operatorname{sgn}(c_{j-1}^*) - \operatorname{sgn}(c_j^*)] \quad \text{if} \quad A_j^* \neq 0. \tag{1.3}$$

If $\gamma_j\gamma_{j-1} > 0$ then $c_j^* c_{j-1}^* > 0$ and (1.3) cannot hold. Therefore (ii) is assured. One now obtains (iii) by observing from (1.3) that if $\gamma_j > 0$ and $\gamma_{j-1} < 0$ then $A_j^* \leq 0$, if $\gamma_j < 0$ and $\gamma_{j-1} > 0$ then $A_j^* \geq 0$.

Remark 1. Note that the conclusions (ii) and (iii) of Proposition 1.4 only depend on $c_i^* c_{i-1}^*$ not being 0. A consequence of (ii) of Proposition 1.4 is that $\gamma_{j-1}, \gamma_j, \gamma_{j+1} > 0$ implies $A_j^* = A_{j+1}^* = 0$ which implies that $c_j^* = \gamma_j$. The same conclusion holds if all three γ's are < 0.

We now give some illustrative examples. A simple computational program is not yet available but the examples indicate a wide variety of possible behavior in the context of this section. The notation $\rho = (nM^2/\sigma^2)$ from Proposition 1.4 is used throughout.

Example 1.1. Let $\Gamma f = \sum_1^N f(x_j)/N$. From Proposition 1.2 the best approximate design apportions n/N observations to each site and estimates Γ by $(1/N) \sum_{j=1}^N \bar{Y}(x_j)$ where $\bar{Y}(x_j)$ is the average of the observations at x. The minimum value for (1.2) is σ^2/n which is the mean square error for estimating α in the finite dimensional linear model $EY_t = \alpha$. In this latter model, any design will give the same mean square error. If C_0 is the design which puts all observations at 0, then $J(C_0)$ will be much larger than $J(C^*)$ (e.g., if $N = 3$ and the x's are $\pm$ 1, 0, $J(C_0) = (\sigma^2/n)[1 + (4\rho/9)]$ compared to $J(C^*) = \sigma^2/n$). Note that for the functional considered here the estimator is the least squares estimator.

If N divides n the approximate design is an exact design. Otherwise, implementation of C^* by an exact design can be done in ad hoc fashion at least for cases where N is modest compared to n by taking proportions of observations as close to the approximate solution as possible. In general, computing the best exact design (minimizing (1.1)) is a formidable task.

EXAMPLE 1.2. Let $\Gamma f = f(1) - f(0)$. Since $C1 = \Gamma 1 = 0$ we can write $Cf = cf(1) - cf(0)$. In the approximate problem $J(C) = 4(\sigma^2/n)c^2 + M^2(1-c)^2$ which is minimized by $c^* = \rho/(4+\rho)$ with $J(C^*) = (\sigma^2/n)(4\rho/(4+\rho))$.

The problem here is that of estimating a bounded mean since, by assumption, $|f(1) - f(0)| \le M$. (It is generally true that boundedness of Γ on $\mathscr{F}_1$ is equivalent to Γ being a contrast). If we think of the least squares estimate in this case to be $\bar{Y}_1 - \bar{Y}_0$ then $J(C_{\text{LS}}) = 4\sigma^2/n$ which is considerably greater then $J(C^*)$ unless ρ is large. The size of the possible improvements over C_{LS} in the case of normal errors is studied by Casella and Strawderman (1981) and, for $\rho < 4$, there are substantial improvements possible. For $\rho = 16$, $J(C^*)/J(C_{\text{LS}}) = .8$, and for larger ρ the boundedness problem for estimation begins to disappear.

EXAMPLE 1.3. Let Γ be the contrast $\Gamma f = f(-1) - 2f(0) + f(1)$. For the approximate problem we write the general C as $Cf = af(-1) - (a+b)f(0) + bf(1)$ and minimize

$$J(C) = (\sigma^2/n)(|a| + |b| + |a+b|)^2 + M^2(|1-a| + |1-b|)^2.$$

From Proposition 1.3 one has $0 \le a, b \le 1$ and this reduces $J(C)$ to

$$(4/n)\sigma^2(a+b)^2 + M^2(2 - (a+b))^2.$$

There is a range of optimum choices: take $a + b = 2\rho/(4+p)$ subject to $a \le 1$ and $b \le 1$. For small ρ ($\rho < 4$) one can even have a design with $b = 0$ i.e., $a = 2\rho/(\rho+4)$ with no observations at 1.

EXAMPLE 1.4. Let $\Gamma f = \sum_{j=1}^N \gamma_j f(x_j)$ where γ_j is negative for $j \le r$ and γ_j is positive for $j > r$. This is the simplest class of examples not covered by Proposition 1.2.

If n is large enough then, according to Proposition 1.4, every c_i^* differs from 0 and all $A_j^* = 0$ except possibly for $j = r+1$. Since $A_j^* = 0$, $A_{j+1}^* = 0$ implies $c_j^* = \gamma_j$, we get all $c_j^* = \gamma_j$ except possibly, for c_r^*, c_{r+1}^* with $c_r^* + c_{r+1}^* = \gamma_r + \gamma_{r+1}$. C^* is then easily determined.

For small n use Proposition 1.3 to consider only those C's for which $a_i = c_i - \gamma_i \ge 0$, $i \le r$, and $a_i \le 0$ for $i > r$. Then, with $L = \sum_1^N \gamma_j$, the problem can be reduced to finding

$$\min_{0 < c_q \le \gamma_q, p \le r, q \ge r+1} (\sigma^2/n)\left[\left(2c_q + 2\sum_{q+1}^N \gamma_j - L\right)^2 + \rho\left(c_q(x_q - x_p) + \sum_p^q \gamma_j(x_p - x_j)\right)^2\right].$$

In case $\Gamma f = -2f(1) + f(2) + f(3)$ we find that if $p = 1$, $q = 2$, the c_2 which globally minimizes the above expression is $(\rho - 4)/(4 + \rho)$, so that, when $\rho > 4$, this is the right solution and we get $c_1^* = -2\rho/(4 + \rho)$ and $c_3^* = 1$. For example, if $\rho = 12$ this implies that $n/2$ observations are at 1, $n/6$ observations at 2, $n/3$ observations at 3. If $p < 4$ we have to use $p = 1$, $q = 3$ and get global minimum at $3\rho/(2 + 2\rho)$ which is < 1 if $\rho < 2$. Therefore $c_1^* = -3\rho/(2 + 2\rho)$, $c_2^* = 0$, $c_3^* = 3\rho/(2 + 2\rho)$ if $\rho < 2$. When $2 \le \rho \le 4$, $c_1^* = -1$, $c_2^* = 0$, $c_3^* = 1$ is the solution and

$$\begin{aligned} J(C^*) &= 16\rho/(\rho + 4) & \rho &> 4 \\ &= 4 + \rho & 2 \le \rho &\le 4 \\ &= 9\rho/(1 + \rho) & \rho &< 2. \end{aligned}$$

2. $\mathscr{F}_2$, Discrete parameters. The regression functions in $\mathscr{F}_2$ are smoother than those in $\mathscr{F}_1$ and, while this means that observations carry more information, we also experience more complications in carrying out a development parallel to that in Section 1. While existence of optimum designs still holds (Propositions 2.1 and 2.3) we cannot limit the support of the design in the same way we did in Proposition 1.1. However, in Proposition 2.3, we obtain some information to enable an attack on the approximate problem. Proposition 1.2 has its counterpart in Proposition 2.2.

Consider a functional C with finite support $\{t_1, \cdots, t_k\}$. The space $\mathscr{F}_2$ contains all linear functions so C cannot minimize (0.1) or (0.2) unless

$$C1 = \textstyle\sum_{i=1}^k c_i = \Gamma 1 = \sum_{j=1}^N \gamma_j, \quad Cx = \sum_{i=1}^k c_i t_i = \Gamma x = \sum_{j=1}^N \gamma_j x_j \tag{2.1}$$

for, otherwise, $\sup_{f \in \mathscr{F}_2}(C(f) - \Gamma(f)) = +\infty$.

As in Section 1, let $\{z_1, \cdots, z_m\} = S(C) \cup S(\Gamma)$ and set

$$D(u) = \textstyle\sum_{i=1}^k c_i(u - t_i)I_{(t_i, z_m]}(u), \quad G(u) = \sum_{j=1}^N \gamma_j(u - x_j)I_{(x_j, z_m]}(u). \tag{2.2}$$

Then we see that

$$\begin{aligned} \sup_{\mathscr{F}_2} \int_{z_1}^{z_m} f(t)d(C - \Gamma) &= \sup_{\mathscr{F}_2^0} \int_{z_1}^{z_m} f''(t)[D(t) - G(t)]\, dt \\ &= M \int_{z_1}^{z_m} |D(t) - G(t)|\, dt \end{aligned}$$

so the exact criterion is

$$J(k, \mathbf{n}, \mathbf{t}, \mathbf{c}) = \sigma^2 \textstyle\sum c_i^2/n_i + M^2\left(\int_{z_1}^{z_m} |G - D|\right)^2. \tag{2.3}$$

For C with finite support we set

$$J(C) = \frac{\sigma^2}{n}\left[(\textstyle\sum_{i=1}^k |c_i|)^2 + \rho\left(\int_{z_1}^{z_m} |G - D|\, du\right)^2\right] \tag{2.4}$$

and the approximate problem is then to minimize (2.4) subject to (2.1). As was done at (1.2) we consider $J(C)$ to be defined for finitely supported C's only.

PROPOSITION 2.1. *If $n \geq 2$ there is an optimum solution to the exact problem* (2.3). *If $k \geq 2$ there is an optimum solution to the approximate problem* (2.4) *among all C having at most k points of support.*

PROOF. As in Proposition 1.1, one holds the c_i's fixed so that the variance term of (2.3) or (2.4) is unchanged while the bias term is manipulated. This brings about a reduction to those C which satisfy $-\Delta \leq t_1 \leq \cdots \leq t_k \leq \Delta$ for a suitable Δ. The conclusions of the proposition follow quickly once this reduction is found; further details may be examined in Sacks and Ylvisaker (1982).

For the problem at (2.4) it is not yet clear that a lid can be put on the number of support points of an optimum C, i.e., that an optimum C exists among all finitely supported functions. However it will follow from Proposition 2.3 that if C^* is optimum among all C having at most $2N$ points of support, then C^* is optimum for (2.4). The remainder of the section deals with the solution to (2.4).

PROPOSITION 2.2. *If Γ is a positive measure it is uniquely optimum for* (2.4). *Otherwise, Γ is not optimum.*

PROOF. The first statement is argued exactly as it was in Proposition 1.2. The converse follows from comparisons covering the cases $N = 2$ and $N > 2$ separately (see Sacks and Ylvisaker, 1982 for details).

LEMMA 2.1. *If C is optimum for* (2.4) *among functionals having at most k support points for some $k \geq 2$, then for any s, t in $S(C)$,*

$$\int_s^t \operatorname{sgn}(G - D) = 0.$$

PROOF. The bias term in (2.4) is the only one affected by $\mathbf{t}$. Since

$$\int_{z_1}^{z_m} |G - D| = \int_{z_1}^{t_j} + \int_{t_j}^{z_m}$$

differentiate with respect to t_j to get

$$\frac{d}{dt_j} \int_{z_1}^{z_m} |G - D| = c_j \int_{t_j}^{z_m} \operatorname{sgn}(G - D)\, du.$$

Then, minimizing $\int |G - D|$ subject to $\sum c_i t_i =$ constant leads to the conclusion that $\int_{t_j}^{z_m} \operatorname{sgn}(G - D) =$ constant. This establishes Lemma 2.1.

Let $x < y < z$ be three successive points in $S(C)$ and suppose $S(\Gamma) \cap (x, z) = \phi$. Denote by c_x, c_y, c_z the c coefficients that go with x, y, z respectively. $G(u)$ (see (2.2)) is linear on $[x, z]$ while $D(u)$ is a linear spline on $[x, z]$ with a knot at y. The slope of $D(u)$ on (x, y) is $C(x)$ (recall that $C(x)$ is the distribution function induced by C evaluated at x) and on (y, z) the slope is $C(y)$. Let $A = G - D$.

According to Lemma 2.1, $\int_x^y \operatorname{sgn} A = \int_y^z \operatorname{sgn} A = 0$. Since A is a linear function on (x, y) and on (y, z) this means that $A((x + y)/2) = 0$, $A((y + z)/2) = 0$. Thus, if one of $A(x)$, $A(y)$, $A(z) = 0$ all three are 0 and then A is identically 0 which means that $C(x) = C(y)$ which implies $c_y = 0$. But this contradicts $y \in S(C)$. Assume $A(x) > 0$. Since $A((x + y)/2) = 0$, this means that the slope of A is negative on (x, y) and $A(y) < 0$ so the slope of A is positive on (y, z). Since G has constant slope, $C(x) - C(y) > 0$ and therefore, $c_y < 0$. Alternatively, if $A(x) < 0$ then $c_y > 0$. In fact, as we shall now show, it is impossible that $c_y \neq 0$ at a minimum for J.

LEMMA 2.2. *If C is optimum for* (2.4) *among functionals having at most k support points for some $k \geq 2$, then in any closed interval formed by successive points of $S(\Gamma)$ there are at most two points of $S(C)$.*

PROOF. Assume there are three points as in the paragraph preceding the lemma and that $A(x) > 0$. We will vary c_x, c_y, c_z holding the other c's fixed, the t's fixed and $c_x + c_y + c_z$ and $xc_x + yc_y + zc_z$ constant. These constraints guarantee that $\int 1\, dC = \int 1\, d\Gamma$, $\int t\, dC = \int x\, d\Gamma$, and that $D(u)$ will change only if $u \in [x, z]$. We obtain

$$\begin{aligned}
&\frac{d}{dc_x}\int_{z_1}^{z_m} |G - D|\, du \\
&\quad = \frac{d}{dc_x}\int_x^z |G - D| \\
&\quad = \int_x^y \operatorname{sgn}(G - D)(x - u) + \int_y^z \operatorname{sgn}(G - D)\left[x - u + (y - u)\frac{dc_y}{dc_x}\right] \\
&\quad = \int_x^y \operatorname{sgn}(G - D)(x - u)\, du + \int_y^z \operatorname{sgn}(G - D)\left[-u\left(1 - \frac{z - x}{z - y}\right)\right] du
\end{aligned} \tag{2.5}$$

where we have used $dc_y/dc_x = -(z - x)/(z - y)$ because of the constraints described above and also the fact that $\int_y^z \operatorname{sgn}(G - D) = 0$ (Lemma 2.1). Using the fact that $\operatorname{sgn}(G - D) > 0$ on $(x, (x - y)/2)$, $\operatorname{sgn}(G - D) < 0$ on $((x - y)/2, (y + z)/2)$ and positive again in $((y + z)/2, z)$ we compute the right side of (2.5) to be $(y - x)(z - x)/4 > 0$.

Thus, under the constraints we have imposed

$$\begin{aligned}
\frac{dJ(C)}{dc_x} &= 2\frac{\sigma^2}{n}\left(\textstyle\sum_1^k |c_i|\right)\left(\operatorname{sgn} c_x + \operatorname{sgn}(c_y)\frac{dc_y}{dc_x} + \operatorname{sgn}(c_z)\frac{dc_z}{dc_x}\right) \\
&\quad + 2M^2\left(\int_{z_1}^{z_m} |A|\right)(y - x)(z - x)/4.
\end{aligned} \tag{2.6}$$

The constraints imply that $dc_z/dc_x = (y - x)(z - y)$. Since $c_y < 0$ $(A_y > 0$; see paragraph preceding the lemma) the first term on the right side of (2.6) is nonnegative. Therefore, $dJ(C)/dc_x > 0$ and $J(C)$ cannot be a minimum.

PROPOSITION 2.3. *There exists a* C^* *minimizing* (2.4) *with finite support. Moreover,*

(a) $t_2^* > x_1$, $t_{k-1}^* < x_N$.
(b) $S(C^*) \cap [x_p, x_p+1]$ *contains at most* 2 *points*, $p = 1, \cdots, N-1$.

PROOF. Suppose C is such that $t_1 < t_2 < x_1$. According to Lemma 2.1 and the discussion preceding Lemma 2.2, we either have $A((t_1 + t_2)/2) = 0$ or $J(C)$ can be reduced. If the first alternative holds then, from $A(t_1) = 0$ and $G \equiv 0$ on $[t_1, t_2]$ we get $D \equiv 0$ on $[t_1, t_2]$ and then $c_1 = 0$ which is impossible. Now use Lemma 2.2 to conclude that we need only consider C's with bounded k in which case a C^* minimizing (2.4) exists (see the paragraph following Proposition 2.1) and statements (a) and (b) hold. This completes the proof of Proposition 2.3.

We turn now to the computation of some examples. Earlier results serve to reduce the possible configurations of designs. This together with symmetries, as they appear, enable calculations in examples where there are few points in the support of Γ. For convenience we will adopt the following scheme to denote configurations of design points: Denote a point in $S(C) - S(\Gamma)$ by ○, a point in $S(\Gamma) - S(C)$ by ×, and a point in $S(C) \cap S(\Gamma)$ by ⊗. Thus the scheme ○×○○×○ (read from left to right) denotes a design where $k = 4$, $N = 2$, $t_1 < x_1$, $t_4 > x_2$ and there are two design points in (x_1, x_2).

EXAMPLE 2.1. We take as parameter the simple contrast, $\Gamma f = f(1) - f(-1)$, which is bounded over $\mathscr{F}_1$ (as noted in Example 1.2), but is unbounded here. There is some symmetry which we can use. If $Qf(t) = -f(-t)$ then $\Gamma(Qf) = \Gamma f$. For C satisfying (2.1) set $\bar{C}(f) = (C(f) + C(QF))/2$ and find, by convexity, that $J(\bar{C}) \leq J(C)$. It is enough to consider designs with configurations ○××○, ×○○×, and ○×○○×○ (⊗⊗ is covered as a limiting case).

Take $s > 1$, $C_s f = cf(s) - cf(-s)$ with $cs = 1$ to satisfy (2.1) and consider designs of the first configuration. Note that $D(u) = -c(u + s)$ if $|u| < s$ and that $G(u) = 0$ if $u < -1$, $= -(1 + u)$ if $|u| < 1$, $= -2$ if $u > 1$. Then compute $\int_{-s}^{s} |G - D| = s - 1$ and

$$J(C_s) = (\sigma^2/n)[(2/s)^2 + \rho(s - 1)^2]$$

which is minimized over $s > 1$, by $s^3(s - 1) = 4/\rho$. For configurations of the second type we get the same C_s for $0 < s < 1$ and

$$J(C_s) = (\sigma^2/n)[(2/s)^2 + \rho(1 - s)^2]$$

which for $s \in [0, 1]$ has minimum at $s = 1$ and $J(C_1) = 4(\sigma^2/n) = J(\Gamma)$. Designs of configuration ○×○○×○ can be shown to be worse than Γ. Thus the optimum design is C_s with $s^3(s - 1) = 4/\rho$. As $\rho \to \infty$, $s \to 1$.

$C = \Gamma$ is comparatively inefficient for moderate values of ρ. For example, if $s = 1.3$, $\rho = 6.07$, then $J(C^*)/J(\Gamma) = .73$. The efficiency of Γ gets up to .95 when $\rho \sim 69$ ($s = 1.05$). So, unless M is large compared to σ or n is large, there is considerable advantage in using the optimum C^*.

For an efficiency calculation relative to the linear model $f(x) = \alpha + \beta x$, suppose observations can be taken in $[-2, 2]$. The best design in the straight line model for estimation of $f(1) - f(-1) = 2\beta$ places $n/2$ observations at ± 2 and the least squares estimate has variance σ^2/n. When $\rho = 1/2$ the best design for $\mathscr{F}_2$ is C_2 which takes $n/2$ observations at ± 2. The corresponding estimate is the least squares estimate and $J(C_2) = (\sigma^2/n)(1 + \rho) = 3/2(\sigma^2/n)$. Thus the usual design only retains $2/3$ of its effectiveness in $\mathscr{F}_2$.

EXAMPLE 2.2. Consider the parameter $\Gamma f = f(1) + f(-1) - 2f(0)$. We see that $\Gamma 1 = \Gamma x = 0$ and Γ is bounded over $\mathscr{F}_2$. The symmetry of Γ allows one to look only at C's with $C(t) = C(-t)$. We will show that the optimum configuration is O×⊗×O. We first calculate, for this configuration, the best design. The appropriate C's are of the form $C_s f = cf(-s) - 2cf(0) + cf(s)$ with $c > 0$ and $s > 1$. Since, for this design, $D = c(u + s)$ on $(-s, 0)$ and $G(u) = u + 1$ on $(-1, 0)$ we get (Lemma 2.1) that $\int_{-s}^{0} \operatorname{sgn}(G - D) = 0$ implies $c = 2/s - 1$ (thus $s < 2$). We then calculate $\int_{-s}^{s} | G - D | = s - 1$. Therefore, $J(C_s) = (\sigma^2/n)[(4c)^2 + \rho(s - 1)^2]$ so we have to minimize, over $s > 1$, $16(2/s - 1)^2 + \rho(s - 1)^2$ which gives $\rho s^3(s - 1) + 32s = 64$ ($\rho = 256/27$ implies $s = 3/2$, $\rho \to 0$ implies $s = 2$, $\rho \to \infty$ implies $s \to 1$). Note that $J(\Gamma) = J(C_1) = (\sigma^2/n)\, 16$. For $\rho = 256/27$, $J(C^*)/J(\Gamma) = .26$.

Other possibilities may be ruled out case by case (Sacks and Ylvisaker, 1982).

3. $\mathscr{F}_2$, Derivatives. This section is a short one devoted to parameters of the form $\Gamma f = \sum_1^N \gamma_j f'(x_j)$. Our interest is in the simplest examples since a theory like that in Section 2 follows with no added effort.

We continue to use the notation $Cf = \sum_1^k c_i f(t_i)$. Again, $z_1 < \cdots < z_m$ denotes the combined ordered x_j's and t_i's. In order that $\sup_{\mathscr{F}_2}[Cf - \Gamma f]$ be finite, C must satisfy

$$C1 = \textstyle\sum_1^k c_i = \Gamma 1 = 0, \quad Cx = \sum_1^k c_i t_i = \sum_1^N \gamma_j = \Gamma x. \tag{3.1}$$

If we define D as in (2.2), but replace G in Section 2 by

$$G(u) = -\textstyle\sum_1^N \gamma_j I_{(\gamma_j, z_m]}(u), \tag{3.2}$$

then the arguments leading to Propositions 2.1 and 2.3 go through without further change and we need not restate them.

EXAMPLE 3.1. Let $\Gamma f = f'(0)$. We follow the methods used in Example 2.1 and let $Qf(t) = -f(-t)$. Since $\Gamma f = \Gamma Qf$, we can restrict attention to C's satisfying $Cf = CQf$ and which satisfy $\sum_1^n c_i = 0$, $\sum_1^N c_i t_i = 1$. According to Proposition 2.3 we have only the configuration O×O. Then, the only C's are of the form $C_s f = (1/2s)f(s) - (1/2s)f(-s)$ for $s > 0$. It is easy to compute $J(C_s) = (\sigma^2/n)[(1/s)^2 + \rho(s/2)^2]$ which has minimum value $(\sigma^2/n)\rho^{1/2}$ at $s^* = (4/\rho)^{1/4}$.

EXAMPLE 3.2. Let $\Gamma f = f'(1) - f'(-1)$. Then $\Gamma Qf = -\Gamma f$ so we only consider C's satisfying $CQf = -Cf$, $\sum_1^n c_i = \sum_1^n c_i t_i = 0$. Note that $| \Gamma f | \leq 2M$ so Γ is bounded on $\mathscr{F}_2$.

Consider first the configuration O×OO×O. From symmetry and (3.1) we need only consider $C_{rs}f = cf(s) - cf(r) - cf(-r) + cf(-s)$ for $r < 1 < s$. Lemma 2.1 shows that $r = 2 - s$, $s \leq 2$ and $c(s - 1) = ½$ and let C_s denote the corresponding funtional. Identify $s = 2$ with the configuration ○×○×○ and disregard $s > 2$. A simple calculation then gives $J(C_s) = (4\sigma^2/n)(s - 1)^{-2} + M^2(s - 1)^2$ for $1 \leq s \leq 2$. The minimum of $J(C_s)$ takes place at $s^* = 2$ if $\rho \leq 4$ and at $s^* = (4/\rho)^{1/4} + 1$ if $\rho > 4$. $J(C_{s^*}) = (\sigma^2/n)(4 + \rho)$ if $\rho \leq 4$, $= (\sigma^2/n)4\rho^{1/2}$ if $\rho > 4$.

The remaining configuration that is possible is ×○× which corresponds to the functional $C_0 f \equiv 0$. The oddity of estimating Γ without the use of observations is due to the special circumstance of a bounded parameter. We have $J(C_0) = 4M^2 \leq J(C_2) = 4\sigma^2/n + M^2$ provided $\rho \leq 4/3$.

Therefore, the optimum C^* is C_0 if $\rho \leq 4/3$, $= C_2$ if $4/3 \leq \rho \leq 4$, and $= C_{s^*}$ for $\rho > 4$ where $s^* = 1 + (4/\rho)^{1/4}$.

4. $\mathscr{F}_1$, Continuous parameters. The analysis we present here is for the exact case and we also give asymptotic (as $n \to \infty$) results. The approximate problem is inappropriate because, as we shall see, the support of an optimum design is too diffuse to permit more than one observation at each site. Our concern is with positive functionals $\Gamma f = \int_0^1 f(x)\gamma(x)\,dx$ where $\gamma > 0$ and continuous on (0, 1). The interval [0, 1] is chosen only for convenience but the assumption of positivity of γ brings a decided simplification. Although much of what we do for positive γ can be done for, say, the case where γ changes sign once, we reserve a discussion for another time because it involves considerably more detail.

It will be easy to see that an optimum C^* exists which puts mass at n points, one observation at each point. While equations for finding C^* are stated, the solution to these equations is not easily obtained and this leads us to asymptotic solutions which work very well. In the examples which can be directly calculated we observe that there is a particularly simple suboptimal solution ($C°$ at (4.12) below) which has high efficiency over a range of parameters covering all except extreme cases.

Let $z_* = \min(t_1, 0)$ and $z^* = \max(t_k, 1)$. Let

$$G(u) = \int_0^u \gamma(x)\,dx I_{[0,1]}(u) + G(1)I_{(1,z^*]}(u) \tag{4.1}$$

$$D(u) = \textstyle\sum_{i=1}^k c_i I_{(t_i,z^*]}(u).$$

It is straightforward to get the maximum mean square error to be

$$J(k, \mathbf{n}, \mathbf{t}, \mathbf{c}) = \sigma^2 \sum c_i^2/n_i + M^2 \left(\int_{z_*}^{z^*} |G - D|\right)^2 \tag{4.2}$$

by using

$$\textstyle\sum_{i=1}^k c_i = \int_0^1 \gamma(x)\,dx = \Gamma 1. \tag{4.3}$$

Our first observation is that $0 < t_1, t_k < 1$. For, if $t_1 \leq 0$, then, differentiating

(4.2) with respect to t_1, produces

$$2M^2\left(\int |G - D|\right)(-|G(t_1) - D(t_1^+)|) < 0,$$

unless $c_1 = D(t_1^+) = G(t_1) = 0$. Thus $t_1 > 0$ and similarly, $t_k < 1$. We can now set $z_* = 0$, $z^* = 1$ and, if we set $t_0 = 0$, $t_{k+1} = 1$, then

$$\int_0^1 |G - D| = \textstyle\sum_{i=1}^k \displaystyle\int_{t_i}^{t_{i+1}} |G - D|. \tag{4.4}$$

Differentiating (4.4) at t_i, $1 \leq i \leq k$, produces

$$|G(t_i) - D(t_i^-)| - |G(t_i) - D(t_i^+)|$$

which must be 0 or we can decrease J by holding the c's fixed and moving the t's. Thus

$$G(t_i) = (D(t_i^-) + D(t_i^+))/2. \tag{4.5}$$

Since $D(t_1^-) = 0$, $D(t_1^+) = c_1$ and $G(t_1) > 0$ we get $c_1 > 0$. Since

$$\int_0^1 \gamma > G(t_k) = \textstyle\sum_{i=1}^k c_i - \dfrac{c_k}{2} = \displaystyle\int_0^1 \gamma - \frac{c_k}{2},$$

we have $c_k > 0$.

Let $D_i = D(t_i^+) = D(t_{i+1}^-)$. Then $D_i = c_i + D_{i-1}$ and (4.5) can be written as $G(t_i) = (D_{i-1} + D_i)/2$. If $c_1, \cdots, c_r > 0$, $c_{r+1} < 0$ then $D_{r+1} < D_r$,

$$G(t_{r+1}) = (D_r + D_{r+1})/2 < D_r.$$

If $c_{r+2} < 0$ as well then

$$G(t_{r+2}) = (D_{r+1} + D_{r+2})/2 < D_{r+1} < (D_r + D_{r+1})/2 = G(t_{r+1})$$

which contradicts G being increasing. Therefore, we have $c_r > 0$, $c_{r+1} < 0$, $c_{r+2} > 0$ which implies $G(u) < D_r$ on (t_r, t_{r+1}) and $G(u) > D_{r+1}$ on (t_{r+1}, t_{r+2}). If we change c_r, c_{r+1} to $c_r - \varepsilon$, $c_{r+1} + \varepsilon$ we leave $\sum c_i$ fixed, reduce $c_r^2/n_r + c_{r+1}^2/n_{r+1}$ and bring G and D closer on (t_r, t_{r+2}). This means that we cannot have any negative c_r's.

Set $t_j^* = G^{-1}((D_{j-1} + D_j)/2)$, $j = 1, \cdots, k$. If $n_j \neq 1$ we create a new design replacing t_j^* by $s_1, \cdots, s_{n_j}$ where

$$G(s_p) = D_{j-1} + ((2p - 1)/2n_j)c_j, \quad p = 1, \cdots, n_j.$$

The new design has sites $t_1^*, \cdots, t_{j-1}^*, \{s_p\}, t_{j+1}^*, \cdots, t_k^*$ with coefficients $c_1, \cdots, c_{j-1}, c_j/n_j, \cdots, c_j/n_j, c_{j+1}, \cdots, c_k$. Neither $\sum c_i$ nor $\sum c_i^2/n_i$ are altered and it may be checked that $\int |G - D|$ is reduced. Confirming that an optimal C^* exists is now easy establishing

Proposition 4.1. *If* $\Gamma f = \int_0^1 \gamma(x)f(x)\,dx$ *with* $\gamma > 0$ *on* $(0, 1)$ *and continuous then an optimal* C^* *exists with* $k^* = n$, $n_i^* = 1$ *and* $c_i^* > 0$.

Taking Proposition 4.1 into account and recalling $c_i = D_i - D_{i-1}$ we write $J = (\sigma^2/n)K$ where

$$K(\mathbf{t}, D) = n \textstyle\sum_{i=1}^{n} (D_i - D_{i-1})^2 + \rho\left[\sum_{i=0}^{n} \displaystyle\int_{t_i}^{t_{i+1}} |G - D_i|\, du\right]^2.$$

Differentiate with respect to D_i and get

$$\frac{\partial K}{\partial D_i} = 2n(2D_i - D_{i-1} - D_{i+1}) + 2\rho\theta\left(-\int_{t_i}^{t_{i+1}} \operatorname{sgn}(G - D_i)\, du\right) \tag{4.6}$$

for $i = 1, \cdots, n-1$ where $\theta = \int_0^1 |G - D|$. It follows that if we want to minimize K subject to $D_n = G(1)$ (equivalent to $\sum_1^n c_i = G(1)$) we have to solve (4.6) together with (4.5). Use (4.5) to calculate

$$\begin{aligned} \int_{t_i}^{t_{i+1}} \operatorname{sgn}(G - D_i) &= -\int_{t_i}^{G^{-1}(D_i)} + \int_{G^{-1}(D_i)}^{t_{i+1}} \\ &= -2G^{-1}(D_i) + G^{-1}\left(\frac{D_i + D_{i-1}}{2}\right) + G^{-1}\left(\frac{D_i + D_{i+1}}{2}\right) \\ &= \xi_i \quad \text{(say)}. \end{aligned} \tag{4.7}$$

We then have to solve

$$-D_{i-1} + 2D_i - D_{i+1} = \rho(\theta/n)\xi_i, \quad i = 1, \cdots, n-1 \tag{4.8}$$

where θ is defined following (4.6), ξ_i is given at (4.7) and $D_0 = 0$, $D_n = G(1)$.

EXAMPLE 4.1. $\Gamma f = \int_0^1 f(x)\, dx$ so $\gamma \equiv 1$ and $G(u) = u$.

$$\xi_i = ½[D_{i-1} - 2D_i + D_{i+1}].$$

Therefore, (4.8) becomes $-D_{i-1} + 2D_i - D_{i+1} = 0$, $D_0 = 0$, $D_n = 1$ which implies $D_i = i/n$ or $c_i^* = 1/n$ and $t_i^* = (2i - 1)/2n$. An easy calculation shows that

$$J(C^*) = (\sigma^2/n)[1 + \rho/16n^2].$$

EXAMPLE 4.2. Let $\Gamma f = \int_0^1 2xf(x)\, dx$ so $G(u) = u^2$. Consider the case $n = 2$ and note that $D_0 = 0$, $D_1 = z$, $D_2 = 1$ with $0 < z < 1$. The problem is to determine z from (4.8). If we let $M^2/\sigma^2 = 6$, then $z = .487$. This translates to the optimum functional $C^*f = .487(.493) + .513f(.862)$. In fact, there is little effect due to M^2/σ^2 in the present example. For the limiting case $M^2/\sigma^2 \to 0$, $z = .5$ and $C^*f = .5f(.5) + .5f(.866)$; for the limiting case $M^2/\sigma^2 \to \infty$, $(4 - \sqrt{2})z^{1/2} = (\sqrt{2}/2)(1 + z)^{1/2}$ at $z = .427$, so $C^*f = .427f(.462) + .573f(.845)$.

An iterative solution to (4.8) is feasible provided n is small. Rather than pursue this direction, we turn to the problem of producing good designs when n is large. In such an asymptotic study there is the effect of the parameter M^2/σ^2 since it controls the balance between variance and squared bias. In the setting of this section it is generally true, as in Example 4.1, that variance and bias are each $O(1/n)$.

In what follows we will suppress the dependence of the D_j's on n and, for simplicity, assume that $G(1) = 1$. We use (4.5), the fact that $n_j = 1$ and the notation $\delta_j = (D_j + D_{j+1})/2$, $t_{j+1} = G^{-1}(\delta_j)$ to write

$$\begin{aligned}
\int_0^1 &| G - D | \, du \\
&= \int_0^{t_1} G(u)\, du + \textstyle\sum_1^{n-1} \displaystyle\int_{t_j}^{t_{j+1}} | G - D_j | + \int_{t_n}^1 (1 - G(u))\, du \\
&= \int_0^{\delta_0} \frac{u\, du}{\gamma(G^{-1}(u))} + \textstyle\sum_1^{n-1} \displaystyle\int_{\delta_{j-1}}^{\delta_j} \frac{| u - D_j |}{\gamma(G^{-1}(u))}\, du + \int_{\delta_{n-1}}^1 (1 - u) \frac{du}{\gamma(G^{-1}(u))} \\
&= \frac{D_1^2}{8} \frac{1}{\gamma(t_1)} + \textstyle\sum_1^{n-1} \displaystyle\frac{(D_j - D_{j-1})^2}{8} \frac{1}{\gamma(t_j)} \\
&\quad + \textstyle\sum_1^{n-1} \displaystyle\frac{1}{8} (D_{j+1} - D_j)^2 \frac{1}{\gamma(t_{j+1})} + \frac{1}{8} (1 - D_{n-1})^2 \frac{1}{\gamma(t_n)} \\
&\quad + o(\textstyle\sum_1^n (D_j - D_{j-1})^2) \\
&= \textstyle\sum_1^n \displaystyle\frac{(D_j - D_{j-1})^2}{4} \frac{1}{\gamma(t_j)} + o(\textstyle\sum (D_j - D_{j-1})^2).
\end{aligned} \tag{4.9}$$

Since $D_j - D_{j-1} = c_j$, $\sum (D_j - D_{j-1})^2 \geq 1/n$ with equality when $c_i = c_i^0 = 1/n$ and we can use the Cauchy/Schwarz inequality on the right side of (4.9) to get

$$\begin{aligned}
\int_0^1 | G - D | &\geq \frac{1}{4n} \left(\sum (D_j - D_{j-1}) \frac{1}{\gamma^{1/2}(t_j)} \right)^2 + o\left(\frac{1}{n}\right) \\
&= \frac{1}{4n} \left(\int_0^1 \frac{du}{\gamma^{1/2}(G^{-1}(u))} \right)^2 + o\left(\frac{1}{n}\right)
\end{aligned} \tag{4.10}$$

where we also use $\max_j (D_j - D_{j-1}) \to 0$ which, if violated, would result in a larger lower bound than given by (4.10). It follows from (4.10) and the lower bound on $\sum (D_j - D_{j-1})^2$ that

$$J(C^*) \geq \frac{\sigma^2}{n} + \frac{M^2}{16n^2} \left(\int_0^1 \frac{du}{\gamma^{1/2}(G^{-1}(u))} \right)^4 + o\left(\frac{1}{n^2}\right). \tag{4.11}$$

If C° denotes the functional with $c_i^\circ = 1/n$ and t_i° determined by (4.5) so that $t_i^\circ = G^{-1}((2i - 1)/2n)$ then, from (4.9),

$$J(C^\circ) = \frac{\sigma^2}{n} + \frac{M^2}{16n^2} \left(\int_0^1 \frac{du}{\gamma(G^{-1}(u))} \right)^2 + o\left(\frac{1}{n^2}\right) = \frac{\sigma^2}{n} + \frac{M^2}{16n^2} + o\left(\frac{1}{n^2}\right). \tag{4.12}$$

(4.11) and (4.12) can be used to show that C° is usually an adequate choice except for extreme G's or when $\sigma = nM^2/\sigma^2$ is substantial compared to n^2.

EXAMPLE 4.3. Let $\gamma(u) = \alpha u^{\alpha-1}$ $\alpha \geq 1$. Then $G(u) = u^\alpha$ and direct calculation and (4.11), (4.12) gives

$$\frac{J(C^*)}{J(C^\circ)} \geq \frac{1 + \dfrac{M^2}{n\sigma^2} \cdot \dfrac{\alpha^2}{(1+\alpha)^4} + o\left(\dfrac{1}{n}\right)}{1 + \dfrac{M^2}{16n\sigma^2} + o\left(\dfrac{1}{n}\right)}.$$

Thus, unless α is large or $M^2/n\sigma^2$ is not small and $\alpha > 1$, the efficiency of C° will be high. For example, if $\alpha = 2$ the efficiency is at least .99 unless $M^2/\sigma^2 \geq .8n$ which means that the bias effect is substantially greater than σ.

In order to minimize the bias term at (4.9) take, for some constant a, $D_j - D_{j-1} = a\gamma^{1/2}(t_j)$ with $D_j = H(j/n)$, H continuously differentiable on [0, 1], $H(0) = 0$, $H(1) = 1$, and $H' = na\gamma^{1/2}(G^{-1}(H))$. Then

$$\text{(4.13)} \qquad \int_0^1 |G - D| = \frac{1}{4n}\left(\int_0^1 \frac{du}{\gamma^{1/2}(G^{-1}(u))}\right)^2 + o\left(\frac{1}{n^2}\right).$$

In order to gauge the behavior of the corresponding C, which we denote by C_B, we have to estimate $\sum (D_j - D_{j-1})^2$.

EXAMPLE 4.4. Continuing with the setup of Example 4.3, we find $H(t) = t^{2\alpha/(1+\alpha)}$ and

$$\sum (D_j - D_{j-1})^2 = \sum_{j=1}^n \left[\left(\frac{j}{n}\right)^{2\alpha/(1+\alpha)} - \left(\frac{j-1}{n}\right)^{2\alpha/(1+\alpha)}\right]^2$$
$$\leq \frac{4\alpha^2}{(1+\alpha)(3\alpha-1)}\frac{1}{n} + \frac{4\alpha^2}{(1+\alpha)^2}\frac{1}{n^2} + o\left(\frac{1}{n^2}\right).$$

Therefore,

$$J(C_B) \leq \frac{4\alpha^2}{(1+\alpha)(3\alpha-1)}\frac{\sigma^2}{n} + \frac{\sigma^2}{n^2}\frac{4\alpha^2}{(1+\alpha)^2} + \frac{M^2}{n^2}\frac{\alpha^2}{(1+\alpha)^4} + o\left(\frac{1}{n^2}\right).$$

If $\alpha = 2$ we get

$$J(C_B) \leq \frac{16}{15}\frac{\sigma^2}{n} + \frac{16}{9}\frac{\sigma^2}{n^2} + \frac{4}{81}\frac{M^2}{n^2} + o\left(\frac{1}{n^2}\right)$$

and then

$$\text{(4.14)} \qquad \frac{J(C^*)}{J(C_B)} \geq \frac{1 + \dfrac{4}{81}\dfrac{\rho}{n^2} + o\left(\dfrac{1}{n^2}\right)}{\dfrac{16}{15} + \dfrac{16}{9n} + \dfrac{4}{81}\dfrac{\rho}{n^2} + o\left(\dfrac{1}{n^2}\right)}.$$

Ignoring the $O(1/n^2)$ terms we can see that, asymptotically, $J(C_B) < J(C^\circ)$ only when M^2/σ^2 is very large, in particular if $M^2/\sigma^2 \geq 81.3n + 135$.

Instead of minimizing the bias term separately, we can use (4.9) with

$D_j = H(j/n)$ and get an asymptotic estimate

$$J(C_H) = \sigma^2 \sum_1^n \left(H\left(\frac{j}{n}\right) - H\left(\frac{j-1}{n}\right)\right)^2 + \frac{M^2}{16n^2}\left(\int_0^1 \frac{H'^2(u)}{g(u)}\,du\right)^2 + o\left(\frac{1}{n^2}\right)$$

$$\le \frac{\sigma^2}{n}\int_0^1 H'^2(u)\,du + \frac{M^2}{16n^2}\left(\int_0^1 \frac{H'^2(u)}{g(u)}\,du\right)^2 + o\left(\frac{1}{n^2}\right)$$

$$= Q(H) + o\left(\frac{1}{n^2}\right) \quad \text{(say)}$$

where $g = \gamma(G^{-1}(H))$. The inequality is caused by the possible contribution of a term of $O(1/n^2)$ coming from the estimate of $(1/n)\int_0^1 H'^2(u)$ for

$$\sum (H(j/n) - H((j-1)/n))^2$$

but will be useful for obtaining some insight into the adequacy of $C°$ as a simple suboptimal solution.

We minimize $Q(H)$ by a variational argument to get

$$H'^2 = a(g/(g + 2\theta)) \tag{4.15}$$

for some $a > 0$, $\theta = \lambda \int H'^2/g$, $\lambda = \rho/16n^2$.

EXAMPLE 4.5. Let $\gamma(x) = 3x^2$ so $G(u) = u^3$ and $g(u) = 3H^{2/3}(u)$. (4.15) then leads to solving

$$H'H^{-1/3}(H^{2/3} + p)^{1/2} = \text{constant}, \quad H(0) = 0, \quad H(1) = 1$$

where $p = 2\theta/3$. The solution is

$$H(u) = \{[(1+p)^{3/2}u + p^{3/2}(1-u)]^{2/3} - p\}^{3/2}.$$

Then

$$\int \frac{H'^2}{g} = [(1+p)^{3/2} - p^{3/2}][(1+p)^{1/2} - p^{1/2}] = B_p \quad \text{(say)}$$

and

$$J(C_H) \sim \frac{\sigma^2}{n}\left[\sum \left(H\left(\frac{j}{n}\right) - H\left(\frac{j-1}{n}\right)\right)^2 + \frac{3p}{2}B_p\right]. \tag{4.16}$$

According to Example 4.3 with $\lambda = M^2/16n\sigma^2$,

$$J(C^*) \gtrsim (\sigma^2/n)[1 + 9/16\lambda], \quad J(C°) \sim (\sigma^2/n)[1 + \lambda].$$

If $p = .2$ then $B_p = .7941$, $(3p/2)B_p = .2382$ and $\lambda = .3778$. If $p = .5$ then $B_p = .7679$, $(3p/2)B_p = .576$ and $\lambda = .9767$.

We calculate

$$\int H'^2 = 1.0244$$

when $p = .2$ and, if $p = .5$,

$$\int H'^2 = 1.0491.$$

Then, for $p = .2$, $J(C_H) \sim (\sigma^2/n)1.2626$ while $J(C^*) \sim (\sigma^2/n)1.2125$ and $J(C^*)/J(C_H) \sim .96$. For $p = .5$, $J(C^*)/J(C_H) \sim .95$. Thus, $J(C_H)$ is close to the asymptotic lower bound. Note that $J(C^*)/J(C^\circ) \sim .88, .78$ for $p = .2, .5$. For smaller values of p the efficiencies are closer to 1. Thus when $p = .05$, $B_p = .8530$, $3pB_p/2 = .064$, $\lambda = .0879$ and

$$\frac{J(C^*)}{J(C_H)} \gtrsim \frac{1.0494}{1.0697} = .98 \quad \text{and} \quad \frac{J(C^*)}{J(C^\circ)} \gtrsim .96.$$

(If we had used $\sum_1^n (H(j/n) - H((j-1)/n))^2$ in place of $(1/n) \int H'^2$ then the calculations are virtually the same. For example, when $n = 10$ and $p = .2$, we would replace 1.0244 by 1.0212.)

Note that $p = .2$ corresponds to $\lambda = .3778$ and, if $n = 10$, this means $M^2/\sigma^2 = 60.4$ which is an extreme situation and even then the efficiency of C° is .88/.96 = .92. Thus C° appears to be a reasonable choice.

5. $\mathscr{F}_2$, Continuous parameters. We consider parameters of the form $\Gamma f = \int_0^1 \gamma(x) f(x)\, dx$ with $\gamma > 0$ and continuous on (0, 1). Because of the difficulties in obtaining explicit results we will concentrate mostly on asymptotic solutions. Even here, there are difficulties reflecting those encountered in related approximation theory contexts which we will mention later.

Suppose that n_i observations are taken at sites $t_1 < t_2 < \cdots < t_k$ and put $z_* = \min(0, t_1)$, $z^* = \max(1, t_k)$. A design C must satisfy $CL = \Gamma L$ for any linear function L. Consequently, if we set, as in Section 2,

$$\begin{aligned} G(u) &= \int_0^u (u - x)\gamma(x)\, dx I_{(0,1]}(u) + [(u-1)G'(1) + G(1)] I_{(1,z^*]}(u) \\ D(u) &= \textstyle\sum_{i=1}^k c_i (u - t_i) I_{(t_i, z^*]}(u) \end{aligned} \tag{5.1}$$

we get

$$\sup_{\mathscr{F}_2} |\Gamma f - Cf| = M\left(\int_{z_*}^{z^*} |G - D|\, du\right) \tag{5.2}$$

and the maximum mean square error is

$$J(k, \mathbf{n}, \mathbf{t}, \mathbf{c}) = \sigma^2 \textstyle\sum_1^k \frac{c_i^2}{n_i} + M^2\left(\int_{z_*}^{z^*} |G - D|\right)^2. \tag{5.3}$$

Because we assumed $\gamma > 0$, G is convex, a property which will play a role in later developments. The condition that $\Gamma L = CL$ for all linear functions is the same as

$$\textstyle\sum_1^k c_i = \int_0^1 \gamma, \quad \sum_1^k c_i t_i = \int_0^1 x\gamma(x)$$

or, equivalently, when $z^* = 1$,

$$D(1) = G(1), \quad D'(1) = G'(1) \tag{5.4}$$

($D'(1)$ is left-hand derivative at 1.)

If $\mathbf{c}$ is fixed then minimizing J with respect to the t's leads to the Lagrange problem $\partial J/\partial t_i - \lambda c_i = 0$. Since

$$\frac{\partial J}{\partial t_i} = 2M^2 \int |G - D| \int_{t_i}^{z^*} \operatorname{sgn}(G - D)c_i,$$

we get

$$\int_{t_i}^{z^*} \operatorname{sgn}(G - D) = \lambda'$$

or

$$\int_{t_i}^{t_{i+1}} \operatorname{sgn}(G - D) = 0, \quad i = 1, \cdots, k - 1 \tag{5.5}$$

(compare with Lemma 2.1). If $t_1 < t_2 < 0$ we would get

$$0 = \int_{t_1}^{t_2} \operatorname{sgn}(G - D) = -\int_{t_1}^{t_2} \operatorname{sgn} D = -\int_{t_1}^{t_2} \operatorname{sgn}(c_1(u - t_1))\, du$$
$$= \mp(t_2 - t_1) \neq 0.$$

Therefore we need not consider designs with more than one point to the left of 0 and, similarly, with more than one point to the right of 1. From this it follows easily as in Section 2 that we cannot have $t_1 \to -\infty$ or $t_k \to \infty$ and then an optimum C^* exists.

PROPOSITION 5.1. *If C^* is optimum then $c_i^* > 0$ for all i.*

PROOF. From (5.5)

$$0 = \int_{t_1}^{t_2} \operatorname{sgn}(G - D) = \int_{t_1}^{t_2} \operatorname{sgn}(G - c_1(u - t_1))$$

which implies $c_1 > 0$ because $G \geq 0$. Thus, $c_1^* > 0$ and, similarly, $c_k^* > 0$. Suppose $c_j < 0$ and $c_1, \cdots, c_{j-1} > 0$, $1 < j < k$.

The further assumption that $G(t_j) - D(t_j)$ is nonnegative leads to $G(u) - D(u)$ positive on (t_j, t_{j+1}) in violation of (5.5). Thus $G(t_j) - D(t_j) < 0$ and it readily follows that $G(u) - D(u) < 0$ on $((t_{j-1} + t_j)/2, (t_j + t_{j+1})/2)$ with $G(u) - D(u) > 0$ on $(t_{j-1}, (t_{j-1} + t_j)/2) \cup ((t_j + t_{j+1})/2, t_{j+1})$. Set $x = t_{j-1}$, $y = t_j$, $z = t_{j+1}$ and vary c_{j-1}, c_j, c_{j+1} subject to $c_{j-1} + c_j + c_{j+1}$ and $c_{j-1}x + c_j y + c_{j+1}z$ constant. Calculating as in (2.5) we get

$$\frac{d}{dc_j} J = 2\sigma^2\left[-\frac{(z - y)}{z - x}\frac{c_{j-1}}{n_{j-1}} + \frac{c_j}{n_j} - \frac{(y - x)}{z - x}\frac{c_{j+1}}{n_{j+1}}\right] - \theta(z - y)(y - x)$$

for a positive θ. Now if $c_{j+1} > 0$ we find $(d/dc_j)\, J < 0$, but if $c_{j+1} < 0$ then $G(u) - D(u)$ does not change sign on (t_{j+1}, t_{j+2}). The proposition is thus proved.

REMARK 5.1. If $G(t_j) - D(t_j) > 0$ and there are n_j observations at t_j with $n_j > 1$ we can put 1 observation at $t_j - \varepsilon$ with coefficient c_j/n_j and the rest at $t_j + \varepsilon/(n_j - 1)$ each with coefficient c_j/n_j. Then $\sum c_i^2/n_i$ remains unchanged and (5.4) still holds. If ε is small then the new $|G - D|$ is the same as the old $|G - D|$ except on $(t_j - \varepsilon, t_j + \varepsilon/(n_j - 1))$ where it is smaller. Thus $\int |G - D|$ is reduced and so is J. Based on this we could show that a C for which $G(t_j) - D(t_j) > 0$ for all j, is a candidate for optimality only if $n_j = 1$. It is clear that $G(t_j) - D(t_j) > 0$ for all j means, by virtue of convexity of G and (5.5), that G crosses D exactly twice in (t_j, t_{j+1}). We have been unable to rule out the possibility that for an optimal C, G crosses D only once in some interval (t_j, t_{j+1}) although it appears from examples that we should expect the double crossing to be the common situation.

EXAMPLE 5.1. Let $\gamma(x) \equiv 1$. Then $G(x) = x^2/2$. For minimizing (5.3) when $n = 2$ use symmetry and (5.4) to reduce to considering functionals $C_s f = \frac{1}{2} f(s) + \frac{1}{2} f(-s)$ with $s < \frac{1}{2}$. The design with two observations at $\frac{1}{2}$ is covered as a limiting case. Since $D(s) = 0$ and D has slope $\frac{1}{2}$ on $(s, 1 - s)$, $G - D \le 0$ on $(s, 1 - s)$ if $s \le 0$. Thus, by (5.5), $s > 0$.

For $s \le \frac{1}{4}$ the roots of $G - D$ occur at $\frac{1}{2} \pm \frac{1}{2}\sqrt{1 - 4s}$. Since the distance between these roots must be half the length of $[s, 1 - s]$ for (5.5) to be satisfied, $\sqrt{1 - 4s} = \frac{1}{2}(1 - 2s)$ so $s = \sqrt{3} - \frac{3}{2} = .2321$. If $s > \frac{1}{4}$ then $G - D$ has no roots in $(s, 1 - s)$ which violates (5.5) so reduction to $s \le \frac{1}{4}$ is necessary.

We turn to asymptotic solutions. Here we take all $n_i = 1$ and t_i's $\in [0, 1]$. We first consider C's with $c_i = 1/n$. This guarantees that the variance term is as small as possible and, as seen in Section 4, such C's can be expected to be adequate suboptimal choices. Implicit in looking at such C's is the assumption that $G'(1) = 1$; otherwise we would consider $nc_i = G'(1)$.

Minimizing J with this choice of $\mathbf{c}$ appears difficult. In order to obtain some estimates we will proceed by defining $\mathbf{t}$ so that $G - D$ can be estimated. Accordingly, let $\boldsymbol{\xi}$ be defined by

$$G'(\xi_j) = \int_0^{\xi_j} \gamma(x)\, dx = \frac{j}{n}, \quad j = 1, \cdots, n \tag{5.6}$$

and then define t_j by

$$G(\xi_j) - \frac{\xi_j j}{n} = -\int_0^{\xi_j} x\gamma(x)\, dx = -\Sigma_1^j \frac{t_i}{n}. \tag{5.7}$$

The convexity of G assures that $\xi_{j-1} < t_j < \xi_j$. The motivation here is that $G - D \ge 0$, D is tangent to G at ξ_j. Therefore

$$\int_{\xi_j}^{\xi_{j+1}} |G - D| \le \frac{1}{6} (\xi_{j+1} - \xi_j)^3 \gamma(\eta_j) \quad \text{for some} \quad \eta_j \in (\xi_j, \xi_{j+1}).$$

From (5.6), $\xi_{j+1} - \xi_j = 1/n\gamma(\tau_j)$, $\tau_j \in (\xi_j, \xi_{j+1})$ and we get

$$\int_0^1 |G - D| \le \frac{1}{6n^2} \Sigma_1^n \frac{\gamma(\eta_j)}{\gamma^2(\tau_j)} (\xi_{j-1} - \xi_j) = \frac{1}{6n^2} \int \frac{dx}{\gamma(x)} + o\left(\frac{1}{n^2}\right). \tag{5.8}$$

Since there are cases where $\int_0^1 du/\gamma(u) = +\infty$ we have to exercise some caution to get reasonable estimates in explicit examples provided $1/\gamma$ is integrable and for example, γ has a bounded derivative.

EXAMPLE 5.2. Let $G(u) = u^2/2$. Then $\xi_j = j/n$, $t_j = (2j - 1)/2n$ and $\int |G - D| = 1/6n^2$ giving $J = \sigma^2/n + M^2/36n^4 + o(1/n^4)$.

If $G(u) = u^3/3$ then $\xi_j = (j/n)^{1/2}$ and $t_j = ⅔(j^{3/2} - (j - 1)^{3/2})/n^{1/2}$ and then $\sum (\xi_{j+1} - \xi_j)^3\gamma(\eta_j) \sim (\log n)/4n^2$ so

$$J \sim \frac{\sigma^2}{n} + \frac{M^2}{(24)^2}\frac{(\log n)^2}{n^4}.$$

If $G(u) = u^4/4$, $\xi_j = (j/n)^{1/3}$, $t_j = ¾(j^{4/3} - (j - 1)^{4/3})/n^{1/3}$ and $\sum (\xi_{j+1} - \xi_j)^3\gamma(\xi_j) \sim 1/3n^{5/3}$ then

$$J \sim \sigma^2/n + (M^2/324)n^{-10/3}.$$

The last two instances in Example 5.2 indicate why using $\int 1/\gamma$ may be inappropriate. Unless G has zero of very high order at 0 we are inclined to the use of the design defined by (5.6), (5.7). Although the choice of t_j at (5.7) isn't quite correct, it should suffice for most purposes since the best bias term obtainable is $O(n^{-2})$ as indicated by the approximation theory results of Pence and Smith (1982).

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DEPARTMENT OF MATHEMATICS
NORTHWESTERN UNIVERSITY
EVANSTON, ILLINOIS 60201

DEPARTMENT OF MATHEMATICS
UNIVERSITY OF CALIFORNIA
LOS ANGELES, CALIFORNIA 90024