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ESTIMATING SOLUTIONS OF FIRST KIND INTEGRAL EQUATIONS WITH NONNEGATIVE CONSTRAINTS AND OPTIMAL SMOOTHING*

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Abstract. A method is presented for estimating solutions of Fredholm integral equations of the first kind, given noisy data. Regularization is effected by a smoothing term which is the L^2-norm of the estimate. We propose a scheme by which an approximately optimal amount of smoothing may be computed, based only on the data and the assumed known noise variances. Numerical examples are given for estimating inverse Laplace transforms.

1. Introduction. In many branches of science, problems arise in which it is desired to solve integral equations of the first kind. This paper presents (a) an estimate of the solution when nonnegative constraints and a particular choice of smoothing are employed, and (b) a data-dependent method by which an approximately optimal amount of smoothing may be chosen.

1.1. Ill-posed problems. To introduce the mathematical problem more specifically, assume that we are given N discrete measurements g_i taken at various points y_i; these are noisy versions of an integral of the product of a known kernel $k(y, x)$ and an unknown function $f^0(x)$. That is, we have

$$g_i = g(y_i) = \int_D k(y_i, x) f^0(x)\, dx + \varepsilon_i, \qquad i = 1, \cdots, N, \tag{1}$$

where ε_i is the random noise associated with the ith measurement, and D is the domain appropriate to the physical situation. The problem is to estimate the unknown function f^0 by some function f which depends on the observed data. This problem is known to be ill-posed; since radically different f^0's could have given rise to very similar data, there is always the danger that small random variations in the data will cause unacceptably different estimates $f(x)$ of $f^0(x)$. This danger follows heuristically from the fact that high frequency components in the true f^0 will be highly attenuated in their contribution to the data g, depending on the smoothness of the kernels.

Subsequent to theoretical work on the properties of ill-posed inverse problems by Tikhonov (1943) and by Lavrentiev (as collected in 1967), a method of obtaining practical solutions of such problems was presented by Tikhonov (1963) as well as by Phillips (1962) and by Twomey (1963). In place of a straightforward inversion of the noisy data of (1), (e.g., by a standard pseudoinverse) producing a wildly oscillatory solution, these authors presented a method of smoothing or "regularizing" the solutions. The method essentially requires that the solution f minimize the sum of two quantities. One quantity is the weighted sum of squared residuals (based on the data g_i and respective predictions $\int k_i(x)f(x)\, dx$). The other quantity is one of several quadratic functionals of f, which furnishes the smoothing by causing variations in f to tend to be small. The development of these and other methods are reviewed in several articles (Turchin (1970), Rust and Burrus (1972), Morozov (1973) and Miller (1974)).

One of the chief problems with the above least-squares method is the difficulty of choosing an appropriate level of smoothing. In the reviews, there are discussions of use of a prior statistical knowledge or assumptions about both measurements and answer in

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order to assign a prior level of smoothing. See Hunt (1971) for simple examples. More recently, a data-dependent choice of optimal intensity of smoothing has been attempted by Hilgers (1976), and Wahba (1977).

1.2. Nonnegative constraints. In this paper, we estimate the solution of (1), where we know in advance that f^0 is nonnegative, and hence, our estimate f is constrained to be nonnegative. In contrast to the excessive broadness characteristic of unconstrained estimates of narrow functions f^0, (Dawson et al. (1976)), the use of nonnegativity constraints greatly sharpens the estimates f (Cooper (1974)). Nonnegative functions are an important class with many physical applications, for example, density functions which do take on zero values so as to permit the nonnegativity constraints to bind. The nonnegativity constraint has been applied to problems in physiology by Wagner et al. (1974), and with prior choice of smoothing intensity by Evans and Wagner (1977).

1.3. Our approach. We shall develop our solution in two parts. First, we obtain an approximate solution of (1) by minimizing the sum of squared residuals plus a constant α times the L^2-norm of f; we call this minimizing function f_α. Second, we try to estimate the optimal value of α, depending on the data. This data dependence is important because it is intuitive that different amounts of smoothing may be appropriate to different true answer functions f^0, even with the same statistical properties of the noise. We would have liked to define our criterion of optimality such that for a given datum g, the square error $\mathrm{SE}(\alpha)$

$$\mathrm{SE}(\alpha)=\int_D (f_\alpha(x)-f^0(x))^2\,dx, \tag{2}$$

is minimized with respect to α, the level of smoothing. This is clearly impossible as long as f^0 is unknown; we propose instead to minimize a certain auxiliary function $H(\alpha)$, which, apart from an additive constant, is a systematic overestimator of $\mathrm{SE}(\alpha)$. In addition, the α which minimizes H tends to be larger than the α which minimizes SE. This function $H(\alpha)$ depends only on the data and some statistical properties of the noise. We assume the noises have mean zero, are uncorrelated, and have known variances. The intimate connection between the choice of L^2-norm for smoothing and the quasi-accessibility of the square error for an optimizing criterion will be treated in § 4.1. Finally, we shall give some examples of this technique when the kernel is $e^{-\mu_i x}$ and the domain of x is $[0, \infty)$, i.e., given noisy, discrete values of the Laplace transform, we obtain estimates of the inverse transform.

2. The minimizing solution—fixed smoothing. The weighted sum of squared residuals is defined by

$$\sum_{i=1}^{N} w_i^2\left(\int_D k(y_i, x)f(x)\,dx-g_i\right)^2,$$

where the weights w_i^2 are inversely proportional to the (assumed known) measurement error variances. We scale the weights such that $\sum_{i=1}^{N} w_i^2=N$. If the noise variances are equal, then $w_i=1$ for all i. If the variances are unequal, we observe that the simultaneous transformation $k(y_i, x)\to k(y_i, x)w_i$ and $g_i\to g_iw_i$ leads to a formulation of the residuals wherein the weights are all unity. Without loss of generality, then, we will take $w_i=1$ for all i, with the understanding that the k's and the g's must be scaled if the noise levels are unequal.

Let $k_i(x)$ denote the function $k(y_i, x)$ and $k(x)$ denote the R^N vector-valued function whose ith component is $k_i(x)$. Define the integral operator K by $Kf=$

$\int k(x)f(x)\,dx$. We let $\|\cdot\|$ denote either the Euclidean R^N vector norm or the L^2-norm as appropriate. Let C be the set of (almost) everywhere nonnegative functions in L^2: $C=\{f: f(x)\geqq 0$ a.e., and $\|f\|^2<\infty\}$. With this notation, we may pose the minimizing problem as follows. For (fixed) $\alpha>0$, and data vector g, minimize the functional $\Phi(f)$, where

$$\Phi(f)=\tfrac{1}{2}\{\|Kf-g\|^2+\alpha\|f\|^2\}, \tag{3}$$

with respect to $f\in C$. We begin with

THEOREM 1. *$\Phi(f)$ has a unique minimum, which we denote by $f_{\alpha,g}$* or f_α.

This theorem is an immediate consequence of the convexity of the closed set C, the strictly convex nature of Φ and of the fact that the Hilbert space L^2 is complete. In the special case of $\alpha=\infty$, we define $f_\infty=0$. We let f_0 denote the limit (in L^2), if it exists, of f_α as $\alpha\to 0^+$.

We now proceed to construct the solution. If the functions k_i are all in L^2, then $\Phi(f)$ has a directional (Gateaux) derivative everywhere, which we denote by $\nabla\Phi$. It is easy to check that $\nabla\Phi$ is given by

$$\nabla\Phi=k(x)\cdot(Kf-g)+\alpha f(x), \tag{4}$$

where the dot denotes the Euclidean vector inner product. By the Kuhn-Tucker theory (see for example Goldstein (1967, Theorem 2, page 99)) and by Theorem 1, $f_{\alpha,g}$ is the only point in C such that

$$\int_D \nabla\Phi(x)|_{f_\alpha}(h(x)-f_\alpha(x))\,dx\leqq 0, \tag{5}$$

for all h in C. This translates into the conditions

$$\nabla\Phi(x)=0,\quad \text{for } f_\alpha(x)>0, \tag{6a}$$

and

$$\nabla\Phi(x)\geqq 0,\quad \text{for } f_\alpha(x)=0. \tag{6b}$$

We can interpret (6) as follows: (6a) states that when $f(x)$ is positive, the contribution of $f(x)$ to Φ is at a calculus minimum; small perturbations of $f(x)$ at that x necessarily increase Φ. On the other hand, (6b) states that when $\nabla\Phi(x)>0$, Φ could have been reduced by decreasing f at that x. However, that is precisely when the constraint is binding, $f(x)=0$.

By slightly rearranging (6), we see that $f_\alpha(x)$ is the only function which satisfies the pair of simultaneous equations ($c\in R^N$)

$$f(x)=\max(0, k(x)\cdot c), \tag{7a}$$

$$(Kf-g)+\alpha c=0. \tag{7b}$$

A more convenient form in which to write this solution may be obtained by substituting (7a) into (7b). That is, for a given function $h(x)$, we define $M(h)$ to be the $N\times N$ matrix whose entries are given by

$$M_{ij}(h)=\int_{h>0} k_i(x)k_j(x)\,dx,$$

where we note that the domain of integration is the domain of positivity of $h(x)$. It is immediate that M is positive semidefinite. Consequently, $(M+\alpha I)$ is nonsingular;

define

$$T(h) = (M(h) + \alpha I)^{-1}.$$

With this notation, we may summarize:

THEOREM 2. *f is given by* (7a), *where c is the unique solution of the implicit vector equation $c = T(k \cdot c)g$, or equivalently, where c is the unique solution of the equation $(M(k \cdot c) + \alpha I)c = g$.*

Appendix A provides useful formulas describing the dependence of M and T on the vectors c and g and the scalar α, some of which are required for the optimization of α in the next section. Appendix B describes a numerical search for the vector c.

We add parenthetically that uniqueness in Theorems 1 and 2 means uniqueness in L^2, which only defines f_α almost everywhere (in the sense of Lebesgue measure) as a function of x. In the special case where the functions k_i are all continuous, Theorem 2 provides a natural definition of f_α as a continuous function of x everywhere. In the remainder of this paper, we shall assume that the k_i's, and hence f_α, are continuous.

In closing this section on the minimizing solution of Φ with fixed smoothing, it is important to remark that regardless of α and g, whenever $f_\alpha(x)$ is positive, it is a linear combination of the kernel functions $k_i(x)$. This has significant consequences in terms of what kinds of solutions can be obtained, and what they can possibly look like. For example, in respiratory physiology, the kernel function $k(y, x)$ is often e^{-xy} (Gomez (1963)) or $1/(x+y)$ (Wagner et al. (1974)), which are both sign regular (see Karlin (1968) and Appendix A). In these cases, the function $k \cdot c$ can have no more than $N-1$ sign changes, and the domain of positivity of f_α consists of at most $(N+1)/2$ intervals. Hence, f_α can have at most $(N+1)/2$ "bumps".

3. An optimal amount of smoothing.

3.1. The approach. As remarked in § 1, a minimization of the square error given in (2) would have been our preferred goal. However, since $f^0(x)$ is unknown, the function SE(α) is also unknown and hence, cannot be explicitly minimized. Instead, we shall simply assert our optimization procedure, and appeal to intuition and some empirical results in §§ 4.3 and 4.4. First, we note that as far as minimizing the SE with respect to α is concerned, we may disregard the additive constant $\|f^0\|^2$, which appears in (2). That is, let us focus instead on SE*, where († denotes the transpose)

$$\text{(8)} \qquad \begin{aligned} \text{SE}^* &= \|f_\alpha - f^0\|^2 - \|f^0\|^2 \\ &= g^\dagger TMTg - 2\int_D f_\alpha(x) f^0(x)\,dx, \end{aligned}$$

and where we have used the notation of Theorem 2 in evaluating $\|f_\alpha\|^2$. Denote the domains of positivity of f_α and f^0 by D_α and D^0, respectively. The cross product term then becomes

$$-2\int_{D_\alpha \cap D^0} f_\alpha(x) f^0(x)\,dx = -2c \cdot \int_{D_\alpha \cap D^0} k(x) f^0(x)\,dx.$$

Now, since our answer function $f_\alpha(x)$ is expected to be a "smoothed" version of the true $f^0(x)$, we might anticipate that D_α would contain D^0. The question of when this "domain containment" occurs will be explored more fully in § 4.2. For the moment, then, let us assume that $D^0 \subseteq D_\alpha$. In this case, $D_\alpha \cap D^0 = D^0$, and the cross product term in (8) becomes

$$-2c \cdot \int_{D^0} k(x) f^0(x)\,dx = -2c \cdot g^0,$$

where g^0 is the "noise-free" datum

$$g^0 = Kf^0.$$

Using the notation of (1) (i.e., $g = g^0 + \varepsilon$), we may then write (assuming domain containment $D^0 \subseteq D_\alpha$),

$$\mathrm{SE}^*(\alpha) = g^\dagger TMTg - 2g^\dagger Tg + 2\varepsilon \cdot c. \tag{9}$$

We now see a possible resolution of the quandary arising from our complete lack of knowledge about f^0 (other than its property of nonnegativity). That is, despite our ignorance, we observe that f^0 affects the SE only through (a) an additive term ($\|f^0\|^2$) which is α independent (and thus is irrelevant to the minimization of the SE with respect to α) and (b) through g^0, or equivalently, through the noise vector ε. In other words, we have traded our lack of knowledge about f^0 for an expression involving the unknown ε (9). However, we are assuming that we know something a priori about the properties of ε, namely their means and variances, and that they are uncorrelated:

$$\mathscr{E}(\varepsilon_i) = 0, \qquad \mathscr{E}(\varepsilon_i\varepsilon_j) = \begin{cases} 0, & i \neq j, \\ \sigma_i^2, & i = j, \end{cases} \tag{10}$$

where $\mathscr{E}$ denotes the expectation value. It is the assumption that we may know the numbers appropriate in (10) (e.g., from the manufacturer's booklet describing the measuring instrument or from experience at replicating data points) that allows us to approach the SE on a solely data-dependent basis.

At this point, we now remark that choosing α by whatever rule is equivalent to dealing somehow with the unknown noise vector ε in (9). Our approach is basically conservative, in the sense of tending to oversmooth, and consists of finding a minimum of an auxiliary function $H(\alpha)$, defined by

$$H(\alpha) = g^\dagger TMTg - 2g^\dagger Tg + 2\varepsilon^* \cdot c, \tag{11}$$

where ε^* is chosen as follows. First, it is natural to take the squared length of ε^* to be the same as the a priori known expected squared length of ε:

$$\|\varepsilon^*\|^2 = \mathscr{E}\|\varepsilon\|^2 = N\sigma^2, \tag{12}$$

where for convenience we have taken the noise variances σ_i^2 to be equal. (See the remark on residual weighting in §2.) Second, we must choose a direction for ε^*. We observe that SE* is maximized (minimized) with respect to ε when ε is parallel (anti-parallel) to the vector c. Our conservative bias suggests then that we take ε^* parallel to c for use in (11). This direction plus the chosen length given in (12) leads to our final auxiliary function,

$$H(\alpha) = g^\dagger TMTg - 2g^\dagger Tg + 2\sigma\sqrt{N}\|c\|. \tag{13}$$

The value of α that minimizes $H(\alpha)$, α_{opt}, will be our optimal choice of the level of smoothing. We may state this criterion more simply by writing

$$\alpha_{\mathrm{opt}} = \arg \min_{\alpha \geqq 0} \max_{\varepsilon} SE(\alpha, \varepsilon\cdot), \qquad \|\varepsilon\|^2 = N\sigma^2, \quad \text{for } D^0 \subseteq D_\alpha. \tag{14}$$

When $D^0 \not\subset D_\alpha$, our α_{opt} (given by minimizing $H(\alpha)$) approximately satisfies (14). See § 4.2.

3.2. Explicit minimization of $H(\alpha)$. We first note (see Appendix A) that M, T, and c are all differentiable functions of α. We may therefore investigate $H'(\alpha) = dH/d\alpha$ in looking for a minimum. By explicit computation, using Appendix A, we obtain

THEOREM 3. *If g is not the zero vector,*

$$(15)\qquad \begin{aligned} (\tfrac{1}{2})H'(\alpha) &= \alpha g^{\dagger}T^3 g - \sigma\sqrt{N}\frac{g^{\dagger}T^3 g}{\|c\|} \\ &= g^{\dagger}T^3 g\left(\alpha - \frac{\sigma\sqrt{N}}{\|c\|}\right). \end{aligned}$$

Now since $g^{\dagger}T^3 g$ is positive, we must have, at any extremum of H,

$$(16)\qquad H'(\alpha) = 0 \Rightarrow \alpha = \frac{\sigma\sqrt{N}}{\|c\|}.$$

The value of α that minimizes $H(\alpha)$ is given by α_{opt}, and is described in the major point of this paper.

THEOREM 4. *Let S be the convex set of vectors in R^N in the range of Kf, $S = (v : v = Kf, f \in L^2, f \geqq 0$ a.e.$)$, and let $\bar{S}$ be the closure of S. If $g \in \bar{S}$, define $g^* = g$; if $g \notin \bar{S}$, let g^* be the closest point in $\bar{S}$ to g. In finding the α that minimizes H, we distinguish three cases:*[1]

(a) *For the signal-to-noise ratio $\|g\|^2/N\sigma^2 > 1$ and for $\|g - g^*\| < \sigma\sqrt{N}$, there is a unique minimum of H at α_{opt} given by*

$$(17)\qquad \alpha_{\text{opt}} = \frac{\sigma\sqrt{N}}{\|c\|}.$$

(b) *For the signal-to-noise ratio $\|g\|^2/N\sigma^2 > 1$ and for $\|g - g^*\| \geqq \sigma\sqrt{N}$, H is strictly increasing, and so*

$$(18)\qquad \alpha_{\text{opt}} = 0.$$

(c) *For $\|g\|^2/N\sigma^2 < 1$, $H(\alpha)$ is monotonically decreasing with α, and so $\alpha = \infty$ is optimal, or equivalently, $f_{\alpha_{\text{opt}}} \equiv 0$ is the recovered answer function.*

Proof. Define

$$(19)\qquad \xi(\alpha) = \alpha^2 g^{\dagger}T^2 g = \alpha^2\|c\|^2,$$

and rewrite (15) as

$$(20)\qquad \left(\frac{1}{2}\right)H'(\alpha) = \left[\frac{g^{\dagger}T^3 g}{\|c\|}\right][\alpha\|c\| - \sigma\sqrt{N}].$$

Hence,

$$(21)\qquad \operatorname{sgn} H'(\alpha) = \operatorname{sgn}(\xi(\alpha) - N\sigma^2).$$

Now differentiating (19), we have

$$\begin{aligned} (\tfrac{1}{2})\xi'(\alpha) &= \alpha g^{\dagger}T^2 g - \alpha^2 g^{\dagger}T^3 g \\ &= \alpha g^{\dagger}T^2 MTg, \end{aligned}$$

which is nonnegative. Therefore, $\xi(\alpha)$ is a monotonically increasing function of α, and (21) implies that $H'(\alpha)$ has at most one sign change. All that remains is to evaluate $\xi(\alpha)$

[1] Case (a) is clearly the most important one, since one expects to find the data g in the range of Kf and to have the signal-to-noise ratio greater than unity.

near $\alpha = 0$ and $\alpha = \infty$. We have, trivially,

$$\lim_{\alpha \to \infty} \xi(\alpha) = \|g\|^2,$$

and so for $\|g\|^2 < N\sigma^2$, (21) together with now strict monotonicity of ξ implies that $H' < 0\ \forall \alpha$, and so has a minimum at $\alpha = \infty$. This proves part (c) of the theorem.

For $\|g\|^2 > N\sigma^2$, we need to evaluate $\xi(0)$. We observe that $\xi(\alpha) = \alpha^2\|c\|^2 = \|\hat{g} - g\|^2$, where $\hat{g} = Kf_\alpha$, and that as $\alpha \to 0$, $\hat{g} \to g^*$, the closest point in $\bar{S}$ to g. (We omit the proof.) Therefore, if $\|g - g^*\|^2 \geqq N\sigma^2$, $\xi(\alpha) > N\sigma^2\ \forall \alpha > 0$, and so by (21), $H' > 0\ \forall \alpha > 0$. This implies that $\alpha = 0$ minimizes H, and completes the proof of part (b). Part (a) follows directly when $\|g - g^*\|^2 < N\sigma^2$ for which $H'(0) < 0$ and monotonicity of ξ implies a unique point such that $H'(\alpha) = 0$, or equivalently $\alpha_{\text{opt}} = \sigma\sqrt{N}/\|c\|$.

4. Discussion and examples.

4.1. Choice of smoothing term. We have chosen the L^2-norm of f as the smoothing term. At first glance, this appears to be quite an arbitrary choice—many other forms suggest themselves (see Tikhonov for example). However, the unique feature of using L^2 is that it produces answers of the form max $(0, k \cdot c)$, and the presence of the kernels in f_α allows one to evaluate (subject to domain containment $D^0 \subseteq D_\alpha$) the cross product term appearing in the square error. Consequently, the problem of optimizing the square error with respect to α is formally a problem involving only the data g and the (noise-free) data g^0. In order to proceed at this point, one must make some a priori assumptions about either f^0 or g^0. We feel that the weaker assumption that we make about g^0, or equivalently ε (10), is preferable to stronger assumptions about f^0. In other words, the quasi-accessibility of the SE, dependent only on g through our weak assumption about ε, removes much of the seemingly ad hoc character of the choice of L^2-norm for smoothing.

4.2. Domain containment. The cross product term in the SE appearing in (8) was evaluated assuming that $D^0 \subseteq D_\alpha$ since we anticipated that this would usually obtain. We further expect that when $D^0 \not\subseteq D_\alpha$, the effect would be negligible. In particular, we shall prove this when f^0 is in the class of functions of the form max $(0, k \cdot c)$. We begin with the cross product term

$$\begin{aligned} -2c \cdot \int_{D_\alpha} kf^0\, dx &= -2c \cdot \int_{D^0} kf^0\, dx + 2I \\ &= -2c \cdot g^0 + 2I, \end{aligned}$$

where

$$I = \left(\int_{D^0} kf^0\, dx - \int_{D_\alpha} kf^0\, dx\right) \cdot c.$$

We wish to show that I is negligible (indeed, if domain containment occurred then I would vanish). We define $D(\alpha, g)$ to be the domain of positivity of $f_{\alpha,g}$. (That is, $D_\alpha = D(\alpha, g)$ and $D^0 = D(0, g^0)$). Let the boundary points of $D(\alpha, g)$ be $\beta_i(\alpha, g)$; define

$$\Gamma(\alpha, g) = \int_{D(\alpha,g)} kf^0\, dx.$$

Then,

$$I = (\Gamma(0, g^0) - \Gamma(\alpha, g)) \cdot c.$$

Our assertion that I is negligible is contained in

THEOREM 5. *If the* $\beta_i(\alpha, g)$ *are twice continuously differentiable functions of* (α, g) *in some neighborhood of* $(0, g^0)$, *then*

$$I = \mathcal{O}(\|g-g^0\|^3+\alpha^3).$$

We shall simply sketch the proof. Let s and t be any of the components of g, or α. Then we have, with the plus or minus sign taken as appropriate for left- and right-hand boundary points,

$$I = \sum_i (\pm) \int_{\beta_i(\alpha,g)}^{\beta_i(0,g^0)} kf^0\,dx \cdot c,$$

$$\frac{\partial I}{\partial t} = \sum_i (\pm)\left\{ f^0k|_{\beta_i(\alpha,g)} \cdot c\frac{\partial \beta_i}{\partial t} + \int_{\beta_i(\alpha,g)}^{\beta_i(0,g^0)} kf^0\,dx \cdot \frac{\partial c}{\partial t}\right\}$$

$$= \sum_i (\pm) \int_{\beta_i(\alpha,g)}^{\beta_i(0,g^0)} f^0k\,dx \cdot \frac{\partial c}{\partial t},$$

since $k \cdot c$ vanishes at $\beta_i(\alpha, g)$. Further, we have

$$\frac{\partial^2 I}{\partial s\partial t} = \sum_i (\pm)\left\{ (f^0k)|_{\beta_i(\alpha,g)} \cdot \frac{\partial c}{\partial t}\frac{\partial \beta_i(\alpha,g)}{\partial s} + \int_{\beta_i(\alpha,g)}^{\beta_i(0,g^0)} f^0k\,dx \cdot \frac{\partial^2 c}{\partial s\partial t}\right\}.$$

(c depends on (α, g) and on β_i in a C^∞ way, so that C^2 assumption on β_i implies c depends on α and g in a C^2 way.)

These formulas allow us to deduce two consequences: (a) At $(\alpha, g) = (0, g^0)$, I and all its partial derivatives of order $\leqq 2$ vanish. This in turn implies that the quadratic Taylor approximation of I expanded about $(0, g^0)$ is identically zero. (b) $\partial^2 I/\partial s \partial t$ is Lipschitz continuous in a vicinity of $(0, g^0)$, i.e., there is a constant C such that

$$\left|\frac{\partial^2 I(\alpha_1, g_1)}{\partial s\partial t} - \frac{\partial^2 I(\alpha_2, g_2)}{\partial s\partial t}\right| \leqq C(\|g_1-g_2\|+|\alpha_1-\alpha_2|),$$

for all (α_1, g_1) and (α_2, g_2) sufficiently close to $(0, g^0)$.

Together, (a) and (b) imply that

$$I(\alpha, g) = \mathcal{O}(\|g-g^0\|^3+\alpha^3).$$

We omit the details of tracking the β_i, their constancy in number for (α, g) sufficiently close to $(0, g^0)$, and their C^∞ differentiability.

We now observe that Theorem 4, together with boundedness of $\|c\| = (g^\dagger T^2 g)^{1/2}$ away from 0 for $\|g^*-g\| < \sigma\sqrt{N}$ imply that

$$\alpha_{\text{opt}} = \mathcal{O}(\sigma).$$

Using this result in Theorem 5 gives us finally the sense in which I is negligible. At optimal α, we have

$$I = \mathcal{O}(\|\varepsilon\|^3+\sigma^3).$$

4.3. Examples. We have computed some results numerically using the Laplace kernel, $k_i(x) = \exp(-\mu_i x)$, $i = 1, \cdots, N$, where $N = 9$ and the μ's run from 0.1 to 10., spaced logarithmically ($\mu_i = 10^{(i-5)/4}$). The noises were picked to be Gaussian, at a relative level of 2%. That is, for each data point, we have

$$g_i = g_i^0 + \varepsilon_i,$$

where ε_i was given by a Gaussian random number generator of mean zero and standard deviation $\sigma_{\text{rel}} g_i^0$, where $\sigma_{\text{rel}} = .02$. The weights, w_i, were picked proportional to $(\sigma_{\text{rel}} g_i)^{-1}$ such that $\sum_{i=1}^{9} w_i^2 = 9$.

The numerical protocol was as follows; for each of four different f^0's:

a. Compute g^0.
b. Add noise to g^0 giving g.
c. For a range of α, compute $f_{\alpha,g}$, $\text{SE}^*(\alpha)$, $H(\alpha)$.
d. Find α_{opt} at the minimum of $H(\alpha)$ and compute $\text{SE}^*(\alpha_{\text{opt}})$.
e. Repeat step (b) through (d) 10 times.
f. From these 10 samples, calculate MSE*, the sample average of SE*, and var(SE*), the sample variance of SE*.

Appendix B describes the actual computational procedure used for finding $f_{\alpha,g}$.

The following four functions were used for f^0:

$$f^0(x) = \begin{cases} \chi_{(.5,5)}(x), \\ \chi_{(.1,.2)}(x) + \chi_{(5,10)}(x), \\ e^{-x}, \\ \delta(x-1), \end{cases}$$

where

$$\chi_{(a,b)}(x) = \begin{cases} 1, & a < x < b \\ 0, & \text{otherwise} \end{cases}.$$

The results are shown in Figs. 1–4. The MSE* is plotted along with error band $\text{MSE}^* \pm (\text{var (SE)})^{1/2}$. Also shown as crosses are the actual square errors obtaining at the α_{opt} for each run.

It is seen that our rule systematically tends to overestimate (by construction) the truly optimal amount of smoothing. This feature is desirable for the following reason. The danger of obtaining a poor estimate of f^0 when oversmoothing is far less than the danger when undersmoothing. This in turn is traceable to the rapid rise in the variance of the SE for α less than the minimizing point of the MSE*.

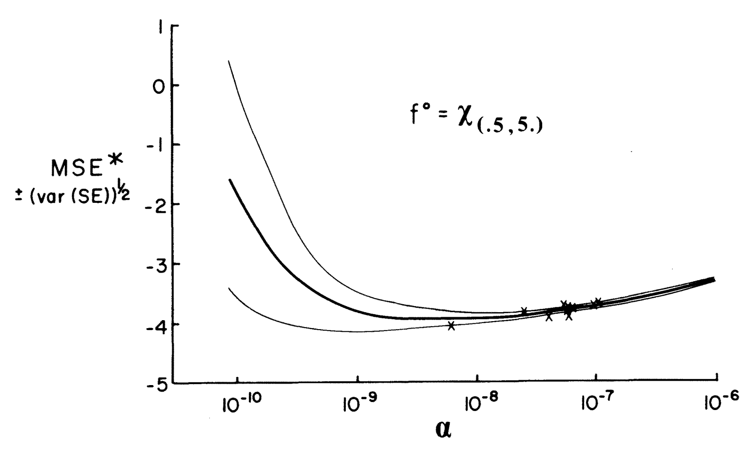

FIG. 1. *The estimated mean square error (average of* $\|f_\alpha - f^0\|^2$*) less* $\|f^0\|^2$ *as a function of* α *over* 10 *trials with* 2% *noise for* $f^0 = \chi(.5, 5)$. *The actual square errors and estimated optimal* α *for each run are shown as* x*'s.*

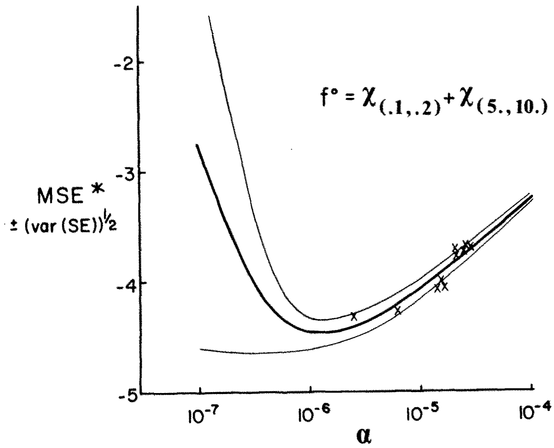

FIG. 2. *Same as Fig.* 1, *for* $f^0 = \chi(.1, .2) + \chi(5, 10)$.

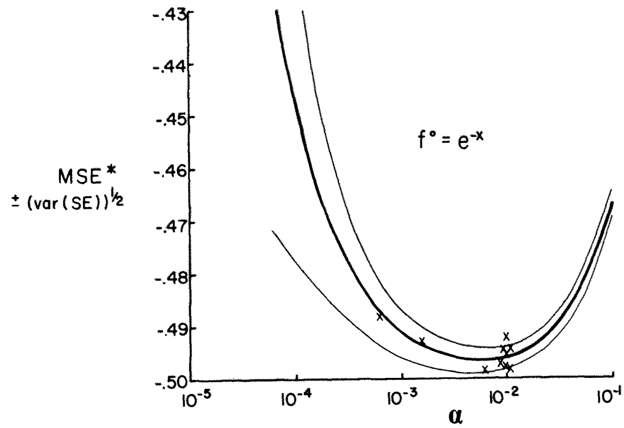

FIG. 3. *Same as Fig.* 1, *for* $f^0 = e^{-x}$.

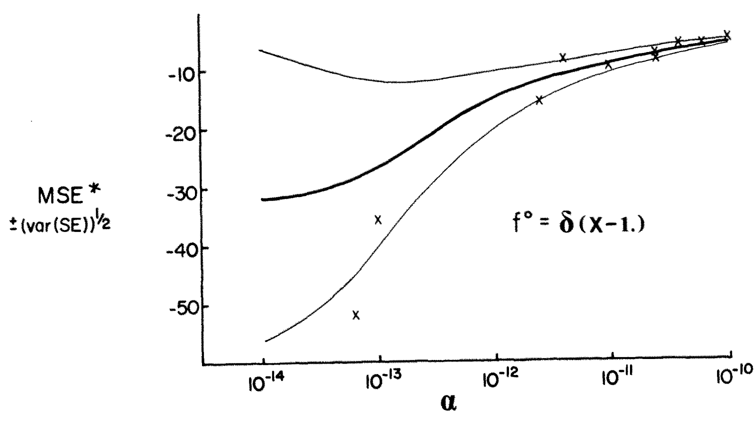

FIG. 4. *Same as Fig.* 1, *for* $f^0 = \delta(x-1)$.

A second feature worth noting is the extreme range of values of α_{opt}. That these four functions f^0 should produce an α_{opt} spread of some ten orders of magnitude argues convincingly for the need for a data-dependent rule for choosing α_{opt}.

Returning to the question of how well our rule works, we show some actual functions recovered. Fig. 5 shows $\chi_{(.5,5)}$ and its equivalent function $f_{\parallel}^0$ in max $(0, k \cdot c)$ space. Fig. 6 shows four typical recoveries using our rule, all of which are quite faithful to $\chi_{(.5,5)}$ (or its equivalent $f_{\parallel}^0$). Similarly, Figs. 7 and 8 show $\chi_{(.1,.2)}+\chi_{(5,10)}$ plus its equivalent $f_{\parallel}^0$ and four typical recoveries. Fig. 9 shows the recovery for exp $(-x)$.

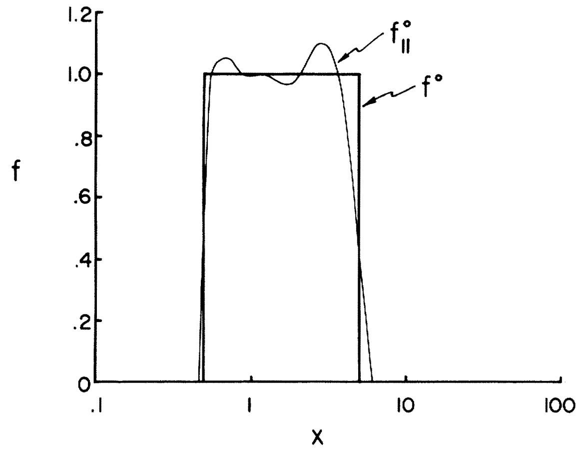

FIG. 5. *The test function $f^0=\chi(.5, 5)$ and that function $f_{\parallel}^0$ of the form* max $(0, k \cdot c)$ *such that $Kf_{\parallel}^0 = Kf^0(=g^0)$.*

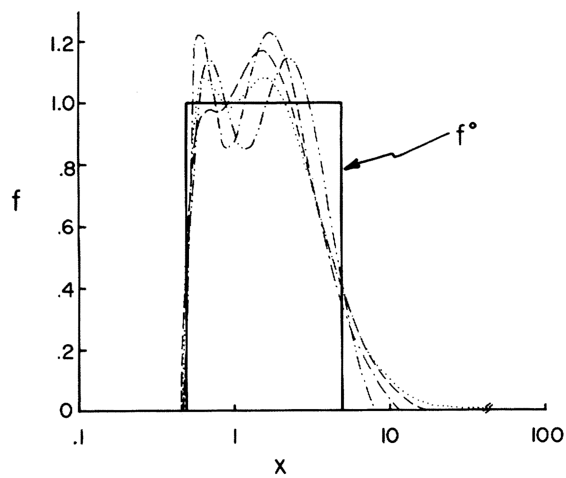

FIG. 6. *Four representative recovered functions f_α at their respectively estimated optimal α. $f^0=\chi(.5, 5)$.*

Displaying recovered answers when f^0 is a delta function is a bit more subtle. That is, f^0 is not in L^2; since $\|f^0\|^2$ is divergent, it does not make sense to talk about how well $f_{\alpha_{\text{opt}}}$ approximates f^0 in L^2. Instead, we may define a measure ν^0 such that $d\nu^0=f^0\,dx=\delta(x-1)\,dx$, and ask how well the measure ν_α, defined by $d\nu_\alpha=f_\alpha\,dx$, corresponds to ν^0. Indeed (we omit the proof), delta functions can be reproduced with noiseless data in the

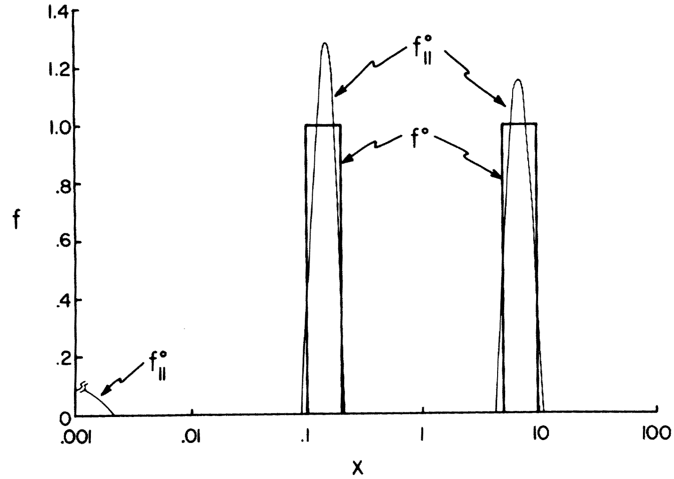

FIG. 7. *Same as Fig.* 5, *for* $f^0 = \chi(.1, .2) + \chi(5., 10)$.

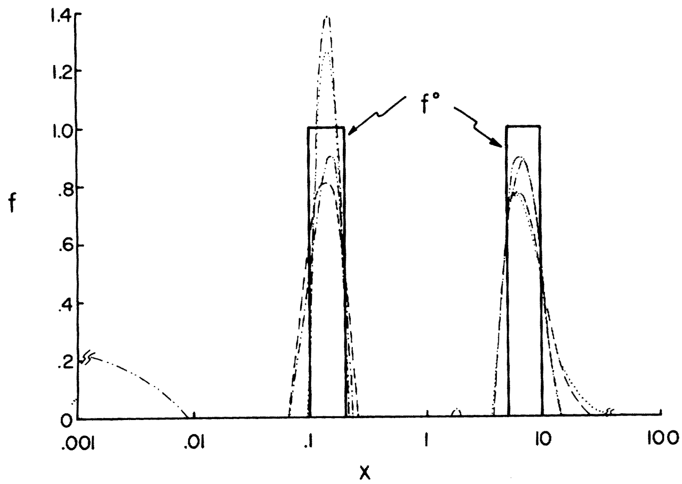

FIG. 8. *Same as Fig.* 6, *for* $f^0 = \chi(.1, .2) + \chi(5., 10)$.

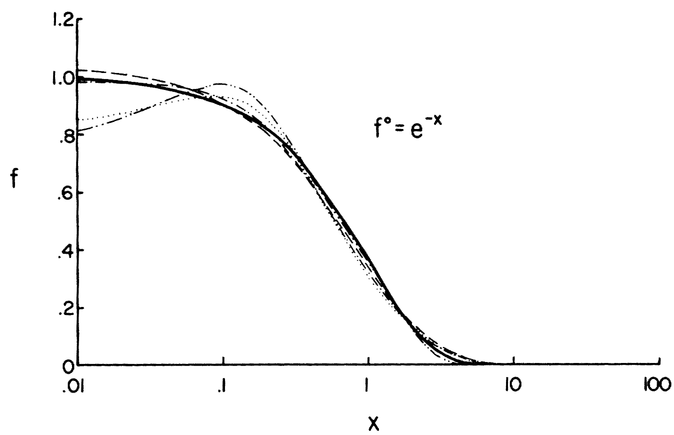

FIG. 9. *Same as Fig.* 6, *for* $f^0 = e^{-x}$.

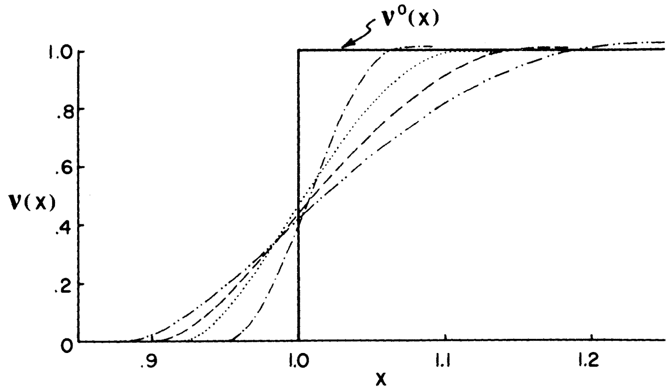

FIG. 10. *Measure* ($\int_0^x f_\alpha(x')\,dx'$) *of four representative recovered functions* f_α *at their respectively estimated optimal* α. $f^0 = \delta(x-1)$.

limit of α tending to zero. Now that is of course an unrealistic limit, but gives us hope that we may still recover functions that are rather narrow. In particular, with ν^0 given by the step function at $x = 1$, Fig. 10 shows the measures $\nu_\alpha(0, x) = \int_0^x f_{\alpha_{\text{opt}}}(x')\,dx'$ for four typical recoveries. We observe first from the fine x scale that they correspond to rather narrow $f_{\alpha_{\text{opt}}}$'s and second, that the total measure of f_α, $\nu_\alpha(0, \infty)$, is indeed very close to unity.

4.4. Picking a rule. Recall that specifying a rule for choosing α_{opt} is in effect making some statement about the $\varepsilon \cdot c$ term in (9), or equivalently by choosing ε^* in (11). For example, we might try setting $\varepsilon^* = 0$, as that is the expectation value of ε. However, a simple calculation shows that $H(\alpha)$ thus defined attains its minimum at $\alpha = 0$. This corresponds to the use of the standard pseudoinverse method to invert (1), and is known to undersmooth drastically the recovered estimate f.

This approach (setting $\varepsilon^* = 0$) was used by Hilgers (1976) in the rather different context of unconstrained optimization. His rule corresponds to seeking a minimum of $H'(\alpha)$, for α finite. If the null space of M is trivial, this occurs at $\alpha = 0$, as remarked above. If, however, null(M) is nontrivial, then $H'(\alpha)$ has its global minimum at $\alpha = \infty$, but may have a local minimum at finite $\alpha > 0$. This latter case defines Hilgers' α_{opt}. We remark, however, that regardless of the character of null(M), $H(\alpha)$ defined by setting $\varepsilon^* = 0$ has its global minimum at $\alpha = 0$.

A remark is in order concerning the relation of our rule to that of Phillips and Twomey. Formally (for $\|g^* - g\| < \sigma\sqrt{N}$), our rule states that $\alpha\|c\| = \sigma\sqrt{N}$, but we note that the residuals

$$\begin{aligned}\|g - Kf_\alpha\|^2 &= \|g - MTg\|^2\\ &= \|\alpha Tg\|^2\\ &= \alpha^2\|c\|^2.\end{aligned}$$

Thus we have, at $\alpha = \alpha_{\text{opt}}$,

$$\begin{aligned}\|g - Kf_{\alpha_{\text{opt}}}\|^2 &= \alpha^2_{\text{opt}}\|c\|^2\\ &= N\sigma^2,\end{aligned}$$

which is formally the same relation used by Phillips and Twomey. However, it must be noted that the overall rule of recovering an answer function from the data includes the choice of which functional to use for the smoothing. Phillips and Twomey both use (continuous or discrete) the L^2-norm of df/dx, which together with the residuals constraint leads to substantial oversmoothing of the recovered answer. Our approach, with $\|f\|^2$ as the smoothing term, leads via the square error to coincidentally the same magnitude of residuals.

As another approach to picking a rule, we might consider expanding SE* about $\varepsilon = 0$ (recalling the dependence of g, M, T, and c upon ε and g^0) up to quadratic terms in ε, and rearranging the result in terms of g and quadratic forms in ε. The latter could then be replaced by their (known) expectation values. Such an expression would be an approximation to an unbiased estimate of MSE*. The resulting rule (i.e., finding an α that minimizes that expression), we have found, tends to oversmooth part of the time, and undersmooth part of the time. However, as we have shown in Figs. 1–4 and argued above, the danger in undersmoothing drastically outweighs that of comparable oversmoothing. The large oscillations that occur with undersmoothing completely swamp out any resemblance f_α might have to f^0.

It is these observations that lead us to believe that our rule is indeed "optimal" in an empirical sense. That is, despite our systematic oversmoothing, the recovered function f_α looks remarkably like f^0 (as seen in Figs. 6, 8, 9 and 10). We argue that such good recovery is the simultaneous result of imposing nonnegativity constraints on f_α and our rule for finding α_{opt}.

Appendix A. In this section, we derive some results that will be helpful in constructing a solution for fixed α as well as in seeking the optimal α. To begin, we assume that the domain D is a real (possibly unbounded) interval, that the kernel $k(y, x)$ is "strictly sign regular" in the sense of Karlin (1968), and that the functions $k_i(x)$ are all N times differentiable. Then for arbitrary c the function $k(x)\cdot c$ has at most $N-1$ roots, and it makes sense to talk about their multiplicities. Further, the domain of positivity of $k(x)\cdot c$ is then the union of finitely many intervals whose endpoints are either roots of $k \cdot c$ or endpoints of D.

DEFINITION. We say the point c in R^N is "good" if

1. $k \cdot c$ has no multiple roots in D,
2. $k \cdot c$ does not vanish at any (finite) endpoints of D, and
3. if D is unbounded,

$$\liminf_{|x|\to\infty} \frac{|k(x)\cdot c|}{\max |k_i(x)|} > 0.$$

(If D is bounded, condition 3 is vacuous.)

Our main result will be that $M(k \cdot c)$ is differentiable with respect to c in the vicinity of any "good" c. This allows us to calculate the derivatives of expressions like $M(k \cdot c)$, $T(k \cdot c)$, etc. These useful formulas will all follow from the following easy consequences of the implicit function theorem:

THEOREM A1. *Let c_0 be "good". Then there is a neighborhood of c_0 in which the roots b of $k(b)\cdot c = 0$ are constant in number, distinct and depend continuously and differentiably on c. The partial derivatives of a root b are*

$$\frac{\partial b}{\partial c_i} = -\frac{k_i(b)}{k'(b)\cdot c}.$$

We thus have formulas valid in neighborhoods of good c's for the matrix elements of $M(k \cdot c)$:

$$M_{ij}(k \cdot c) = \int_D k_i(x)k_j(x)\,dx,$$

where D is the domain of $k \cdot c > 0$.

Note that M depends only on the domain D, and hence, the boundary points b. Furthermore, b is a right-hand boundary point if $k'(b)\cdot <0$ and a left-hand boundary point if $k'(b)\cdot >0$. Straightforward differentiation of this formula, paying attention to the fact that $k(b)\cdot c=0$ for each b, yields

THEOREM A2.

1.
$$\frac{\partial M_{ij}}{\partial c_k}=\sum_b (\pm)\frac{k_i(b)k_j(b)\partial b}{\partial c_k}$$
$$=\sum_b \frac{k_i(b)k_j(b)k_k(b)}{|k'(b)\cdot c|}.$$

2.
$$\sum_j \frac{c_j \partial M_{ij}}{\partial c_k}=0.$$

3.
$$\frac{\partial}{\partial c}(M+\alpha I)c=\frac{\partial G}{\partial c}=M+\alpha I.$$

By the implicit function theorem and Theorem A2 above, we may regard c (and hence, also M, T, and b) as functions of the data g. The following results are then automatic:

THEOREM A3.

1.
$$\frac{\partial (Tg)_i}{\partial g_j}=\frac{\partial c_i}{\partial g_j}=T_{ij}=(M+\alpha I)_{ij}^{-1},$$

and

2.
$$\sum_i \frac{\partial b}{\partial g_i} g_i=0.$$

Lastly, we must include some derivatives with resepct to α. We have

THEOREM A4.

1.
$$\frac{\partial T}{\partial \alpha}=-T\left(\frac{\partial M}{\partial \alpha}+I\right)T,$$

2.
$$\frac{\partial c_i}{\partial \alpha}=\sum_j g_j \frac{\partial T_{ij}}{\partial \alpha},$$

3.
$$\frac{\partial M_{ij}}{\partial \alpha}=\sum_b (\pm)k_i(b)k_j(b)\sum_l \frac{\partial b}{\partial c_l}\frac{\partial c_l}{\partial \alpha}.$$

Using the fact that $k(b)\cdot c=k(b)^{\dagger}Tg=0$, *we have further,*

4.
$$\frac{\partial M}{\partial \alpha}Tg=0,$$

and

5.
$$\frac{\partial c}{\partial \alpha}=\frac{\partial (Tg)}{\partial \alpha}=-T^2 g.$$

Appendix B.

Computational procedure. We seek a procedure for finding f_α, α fixed, where $f_\alpha = k(x)\cdot c$, and c satisfies

$$(M+\alpha I)c = g,$$

where $M_{ij} = \int_D k_i(x)k_j(x)\,dx$, and D is the domain of $k(x)\cdot c > 0$. First, we observe that this is the same problem as finding the minimum of the convex function

$$\psi = (\tfrac{1}{2})c^{\dagger}(M+\alpha I)c - c\cdot g.$$

We have,

$$\psi' \equiv \frac{\partial\psi}{\partial c_i} = \sum_j (M+\alpha I)_{ij}c_j,$$

$$\psi'' \equiv \frac{\partial^2\psi}{\partial c_i \partial c_j} = (M+\alpha I)_{ij}.$$

The algorithm proceeds on the basis of the following iteration (Daniels (1971)). Given a point $c_i \in R^N$ and a direction $\Delta \in R^N$, we compute

(B1) $$c_{i+1} = c_i - \gamma s \Delta.$$

The scalar s is defined by

(B2) $$s = \frac{\Delta\cdot\psi'}{\Delta^{\dagger}\psi''\Delta},$$

and γ is the first of $(\frac{1}{2})^0, (\frac{1}{2})^1, (\frac{1}{2})^2, \cdots$, such that

(B3) $$\psi(c_{i+1}) < \psi(c_i),$$

or

(B4) $$\psi'(c_{i+1})\cdot\psi'(c_i) > 0.$$

For a pure Newton search, we pick the direction

$$\begin{aligned}\Delta &= (\psi'')^{-1}\psi' \\ &= (M+\alpha I)^{-1}((M+\alpha I)c - g),\end{aligned}$$

which incidentally yields a scalar factor $s = 1$. However, in some cases (where the domain D of positivity of $k\cdot c$ is small and α is also small), the condition number of $M+\alpha I$ is such that the inversion of $M+\alpha I$ is numerically impossible. In those cases, we set

$$\Delta = (M+\lambda I)^{-1}\psi',$$

where λ is a fixed constant >0 which prevents the condition number from getting too large. This quasi-Newton search converges more slowly, but it still works. The search is typically terminated when

$$\frac{\|(M+\alpha I)c - g\|}{\|g\|} \leqq 10^{-6},$$

an arbitrarily selected tolerance.

Roundoff error was frequently a problem. We observed several cases where $\|(M+\alpha I)c - g\|/\|g\|$ was small but $>10^{-6}$, and we found that despite the occurrence of

$\psi'(c_{n+1}) \cdot \psi'(c_n) > 0$ (meaning we had chopped the distance too far, and were coming back up in ψ), we had $\psi(c_{n+1}) > \psi(c_n)$! If this happened more than three times, the search was terminated, and the value of c (and hence, $f = \max(0, k \cdot c)$) which gave the least value of ψ was taken as the solution.

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