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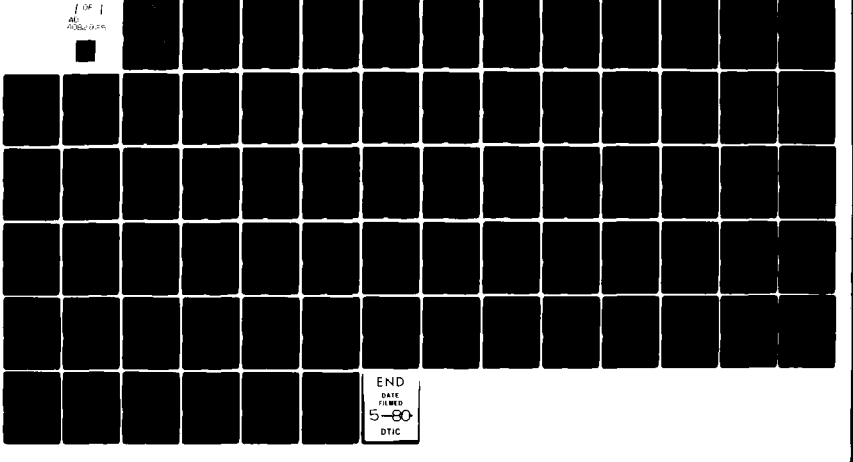

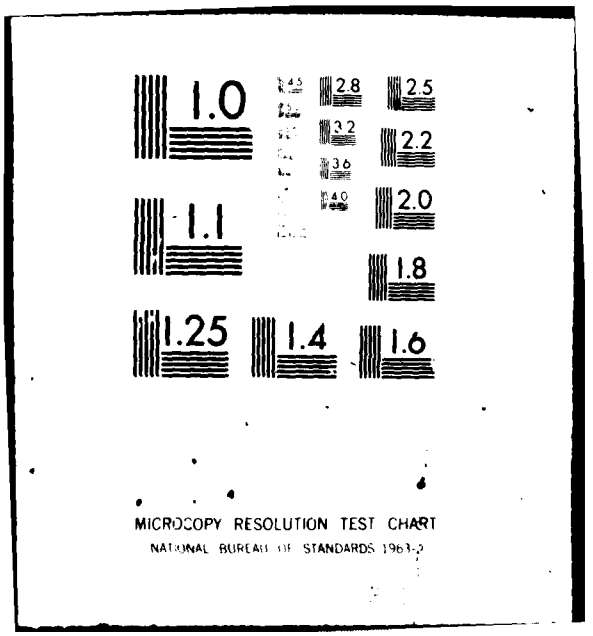
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TECHNICAL REPORT NO. 595

February 1980

ILL POSED PROBLEMS:

NUMERICAL AND STATISTICAL METHODS FOR MILDLY, MODERATELY AND SEVERELY ILL POSED PROBLEMS WITH NOISY DATA

by

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This research supported by the Office of Naval Research under Contract No. N00014-77-C-0675.

Prepared for the Proceedings of the International Conference on Ill Posed Problems, held at Newark, Delaware, October 2-6, 1979. M.Z. Nashed, Ed.

ABSTRACT

We discuss a number of topics related to the practical solution of ill posed problems given noisy data as it might arise in an experimental situation. The model is $z_i = \int_0^1 K(t_i,t)f(t)dt + \varepsilon_i$, $i = 1,2,\ldots,n$, where $z = (z_1,\ldots,z_n)'$ is the data vector, $\varepsilon = (\varepsilon_1,\ldots,\varepsilon_n)'$ is a vector of independent zero mean random variables with common unknown variance, K is known, and it is desired to estimate f given z. We first define the intrinsic rank of the problem where $\int_0^1 K(t_i,t)f(t)dt$ is known exactly. This definition is used to provide insight into the circumstances in which one may expect to estimate f well, moderately well, or poorly. The sensitivity of a regularized estimate of f to the noise is made explicit. After giving the intrinsic rank of the examples of first and second derivative, Abel's equation and Fujita's equation, it is argued that the first three are only mildly ill posed and f should be amenable to accurate estimation by the method of regularization. The method of Generalized Cross Validation (GCV) for choosing the regularization parameter is described and numerical results for the estimation of first and second derivative from noisy data are given. Two numerical algorithms for obtaining a regularized estimate with GCV are detailed. The second uses a B-spline basis to allow the handling of large data sets. Ths use of outside information in the estimation of f is discussed. Three types of outside information are of interest. 1) Several values of continuous linear functionals on f are known approximately, 2) this same information is given exactly and 3) f is known to be in a closed convex set, in particular f non-negative. The GCV estimate of the regularization parameter has to be modified in case 3) if the closed convex set is not a linear manifold. To do this we develop the notion of GCV for constrained problems. Next, we discuss the problem of checking the validity of the "model" K, and provide a crude goodness-of-fit test. Finally we end by describing the (known) result that the number k of iterations in a Landweber iteration for solving large linear systems is a form of regularization parameter. We then show how GCV can feasibly be used to choose k in very large problems like those arising in computerized tomography.

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1. Introduction

We first consider the model

$$z_i = \int_0^1 K(t_i,t)f(t)dt + \varepsilon_i, \quad i = 1,2,\ldots,n, \tag{1.1}$$

where $z = (z_1 \ldots z_n)'$ is the data vector, $\varepsilon = (\varepsilon_1,\ldots \varepsilon_n)'$ is a vector of independent, zero mean random variables with common unknown variance, $K = K(s,t)$ is a known function of two variables and it is desired to recover an estimate of f given the data z. In Sections 2 and 3 f is assumed to be in an abstract Hilbert space H, in Sections 4-7 we assume that H is a reproducing kernel Hilbert space (r.k.h.s.) of functions with specified continuity properties. An estimate of f in (1.1) will be obtained by the method of regularization, by seeking $f \in H$ to minimize

$$\frac{1}{n}\sum_{i=1}^{n}((Kf)(t_i)-z_i)^2 + \lambda||f||^2 \tag{1.2}$$

where $\|\cdot\|$ is a norm or seminorm in H. The smoothing parameter λ will be chosen by the method of generalized cross validation (GCV), and we will consider the insertion of various types of outside information into the minimization, and several algorithmic strategies.

The first goal of this paper is to elucidate and quantify why some ill posed problems can now be solved with "off the shelf" techniques and why others are "impossible". The real issue is, whether the data from the experiment described in (1.1) provides sufficient information concerning f to meet the experimenter's requirements. If so, then the problem can be "solved", usually with the aid of sophisticated mathematical techniques and a powerful computer, and we shall call such problems mildly ill posed. If not, then sophisticated techniques and powerful computers will not provide the missing

information (contrary to uninformed belief!). If the low information content of the experiment can be recognized, then at least two routes are available - a) a redesign of the experiment to provide more information b) the incorporation of a priori or outside information into the solution.

In Section 2 we define the "intrinsic rank" of the experiment described by (1.1). The intrinsic rank of an experiment is the number of linearly independent pieces of information practically available in the data vector z about the function f if there were no errors in the data and K is known perfectly. Examination of the intrinsic rank of a problem can provide valuable information concerning whether or not a satisfactory solution is obtainable. It is computable for the problems we consider in Sections 5 and 6 and should be done routinely.

In Section 3 we discuss the effect of noise on the solution. This is most easily done in terms of what we shall call the canonical representers. The estimated solution will always be in the span of the canonical representers, and so knowledge of them can be a useful diagnostic tool if problems appear. We note here that the intrinsic rank as well as the canonical representers depend on H as well as n, K, and the location of the t_i's.

In Section 4 we give the intrinsic rank, as a function of n, for the examples of first derivative, k^{th} derivative, Abel's equation and Fujita's equation. It can be seen that first and second derivatives, and solutions of Abel's equation should be usefully recoverable with reasonable data sets, while estimation of f by solving Fujita's equation is hopeless in the geometry that we considered.

In Section 5, we first briefly review the method of generalized cross validation (GCV) for choosing λ. We then note some successful experiments in which first and second derivatives were well estimated from noisy data. We propose a method for solving Abel's equation. We note that successful

numerical experiments on Abel's equation have been carried out using a somewhat different approach by Anderson and Jakeman (1975). Next, we describe a "general purpose" algorithm for solving mildly ill posed problems when n is around 25 or 30 up to around 100 or 125. This algorithm, which has its roots in Anselone and Laurent (1968) provides what appears to be a good way of obtaining the minimizer of (1.2) with $||f||^2 = \int_0^1 (f''(u))^2 du$ while simultaneously obtaining the GCV estimate of λ. For n larger than around 130 or so, this algorithm appears difficult to implement on our present system (Univac 1100). We are limited by the necessity to solve $n \times n$ eigenvalue problems. We then borrow an idea from Locker and Prenter (1978a,b), Klein (1979) to suggest that (1.2) be minimized in a B-spline subspace of H. GCV is used to choose λ after the dimension N of the subspace is fixed, and it can also be used to decide between several different N. This approach appears able to handle N up to about 100 with n larger. Algorithmic details are provided.

When a problem is not mildly ill posed, but moderately or severely ill posed, it is generally necessary to make use of outside information to obtain a satisfactory solution. In Section 6 we consider three types of outside information:

1) Values of $L_k f$, $k = 1,2,\ldots$, are known approximately, where the L_k are continuous linear functionals, 2) values of the L_k are known exactly, and 3) f is known to be in a given closed convex set in H. When H is an r.k.h.s., then the set of f satisfying $f(t) \geq 0$, $t \in [0,1]$ is closed convex and this important case is included.

We discuss computing the minimizer of (1.2) using the information 1), 2) or 3). In each case it is to be expected that the optimal λ given the information 1), 2) or 3) will be different than without it. We show how GCV should be applied in each case. In particular, if one minimizes (1.2)

subject to f in a convex set which is not a linear manifold, the solution is not linear in z. It is then necessary to extend the usual GCV method to cover this case. We do that here, and suggest in addition that this extended version can deal with some other nonlinear and robust problems as well.

With the advent of sophisticated techniques for solving ill posed problems, errors in the model, that is, misspecification of K, will increasingly become evident. In Section 7 we make some comments on the detection of serious misspecification in K and tentatively propose an ad hoc goodness-of-fit test which may be used in conjunction with other approaches for checking the model.

In Section 8 we leave Hilbert space and regularization in the form of the minimization of (1.2) to consider extremely large n, say $n > 10^4$, such as occur in computerized tomography. It has been observed by Miller (1974), Fleming (1977), Strand (1976), Bjorck and Elden (1979) that, when a Landweber iteration is used to solve a large linear system approximately, the number of iterations and the constant involved in the iteration play the role of regularization parameters. We show how the number of iterations and the aforementioned constant can be chosen by GCV at a computing cost which is commensurate with the cost of the iteration.

2. The intrinsic rank of an ill posed experimental problem

The intrinsic rank of an ill posed experimental problem as we define it here depends on the following:

i) the operator K.

ii) The number and location of the data points $t_1,\ldots,t_n$.

iii) The space H in which the solution is sought.

iv) The minimum computer roundoff, δ (i.e. $\delta \approx 10^{-14}$ in double precision.)

The intrinsic rank r_I will be the useful number of linearly independent pieces of information about f in the absence of measurement errors, errors in K or cumulative roundoff beyond that in iv).

The effective rank will be less than r_I and will depend on the above as well as

i) σ^2

ii) errors in knowledge of K.

iii) roundoff errors beyond iv) above.

Errors in knowledge of K can be an important source of trouble, we assume K is known accurately until Section 7. We will assume that computer roundoff (iii) can be made negligible compared to experimental error (σ^2) by the use of high quality quadrature formulae, and careful tailoring of the numerical methods used to the intrinsic rank of the problem*. We shall generally ignore it in the discussion. The effect of σ^2 is discussed in Section 3.

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*This means that one avoids division by very small numbers!

We now prepare to define the intrinsic rank r_I of the problem (1.1). We suppose that f is estimated by $f_{n,\lambda}$, the solution to the problem: Find $f \in H$ to minimize

$$\frac{1}{n}\sum_{i=1}^{n}(z_i - \int_0^1 K(t_i,s)f(s)ds)^2 + \lambda||f||^2, \qquad (2.1)$$

where $||f||$ is the norm of f in H. Later we will consider the (usual) case where $||\cdot||$ is a seminorm (for example $||f|| = [\int_0^1 (f''(t))^2 dt]^{1/2}$), however the exposition is considerably simplified with $||\cdot||$ a norm. It is required that H be a space in which the n functionals which map f to $\int_0^1 K(t_i,s)f(s)ds$, $i = 1,2,\ldots,n$, are continuous linear functions. If this is the case, then by the Riesz representation theorem (Akhiezer and Glazman (1961)), there exist n elements $\eta_1,\ldots,\eta_n$, in H called the representers, such that

$$\int_0^1 K(t_i,s)f(s)ds = \langle \eta_i, f\rangle \ , \ f \in H, \ i = 1,2,\ldots,n$$

where $\langle\cdot,\cdot\rangle$ is the inner product in H. For example if $H = L_2[0,1]$ then for fixed i,

$$\eta_i(s) = K(t_i,s) \quad i = 1,2,\ldots,n.$$

If $H = H_R$, the r.k.h.s. with r.k. $R(s,t)$, then

$$\eta_i(s) = \int_0^1 K(t_i,u)R(s,u)du.$$

The reproducing kernel space results we use in this paper can be found in Kimeldorf and Wahba (1971), see also Aronszajn (1950). If H is a finite dimensional space, then each η_i is a linear combination of basis functions.

The solution $f_{n,\lambda}$ to the minimization problem of (2.1) can be written

$$f_{n,\lambda} = \tilde{K}_n^*(\tilde{K}_n\tilde{K}_n^* + n\lambda I)^{-1}z,$$

where $z = (z_1,\ldots,z_n)'$. $\tilde{K}_n$ is the operator which maps H into E_n as follows:

$$\tilde{K}_n f = \begin{pmatrix} \int_0^1 K(t_1,s)f(s)ds \\ \vdots \\ \int_0^1 K(t_n,s)f(s)ds \end{pmatrix}.$$

$\tilde{K}_n^*$ is the adjoint of $\tilde{K}_n$ in the sense that $\tilde{K}_n^*: E_n \to H$, and $\tilde{K}_n^*$ satisfies

$$(z,\tilde{K}_n f) = \langle \tilde{K}_n^* z, f\rangle ,$$

where $(\cdot,\cdot)$ is the Euclidean inner product. It can be verified that $\tilde{K}_n^* z$ has the representation

$$(\tilde{K}_n^* z)(s) = \sum_{i=1}^n z_i \eta_i(s).$$

$\tilde{K}_n\tilde{K}_n^*: E_n \to E_n$ is the operator of multiplication by the $n\times n$ matrix with jk^{th} entry $\langle \eta_j,\eta_k\rangle$. This matrix is the Gram matrix of the representers of the data functionals. If $H = L_2[0,1]$, then

$$\langle \eta_j,\eta_k\rangle = \int_0^1 \eta_j(s)\eta_k(s)ds = \int_0^1 K(t_j,s)K(t_k,s)ds,$$

and, if $H = H_R$, then

$$\langle \eta_j,\eta_k\rangle = \int_0^1\int_0^1 K(t_j,s)R(s,t)K(t_k,t)dsdt.$$

The matrix $(\tilde{K}_n\tilde{K}_n^*)$ is symmetric non-negative definite, and hence has a decomposition

$$(\tilde{K}_n \tilde{K}_n^*) = \Gamma D \Gamma' \tag{2.2}$$

where Γ is an n×n orthogonal matrix and D is a diagonal matrix with eigenvalues (diagonal entries) $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n \geq 0$.

We define the intrinsic rank r_I as the number of eigenvalues λ_i for which $\lambda_i/\lambda_1 > \delta \approx 10^{-14}$ (computer roundoff). Thus r_I is the effective number of linearly independent data functionals in the experiment (1.1) in the absence of experimental errors or errors in K.

We make several observations about r_I. Firstly, if H is a finite dimensional space of dimension N, then $r_I \leq N$. This is reasonable, since, if f is known to be in H, then f is determined by N linearly independent pieces of information, and the experiment (1.1) cannot deliver more. Secondly, if H is a space of functions with several continuous derivatives, then (other things being equal), r_I will be less than if H is L_2. Again, this is reasonable, since, loosely speaking, $\int K(t_i,s)f(s)ds$ and $\int K(t_j,s)f(s)ds$ can be expected to be less linearly independent on smooth functions than on arbitrary elements of L_2.

3. The effect of noise. The canonical representers

Let Γ and $\lambda_1,\ldots,\lambda_n$ be defined by (2.2). We define the canonical data vector $y = (y_1,\ldots,y_n)'$ and the canonical representers $\rho_1,\ldots,\rho_n$ by

$$y = \Gamma' z$$

$$\begin{pmatrix} \rho_1(s) \\ \vdots \\ \rho_n(s) \end{pmatrix} = \Gamma' \begin{pmatrix} \eta_1(s) \\ \vdots \\ \eta_n(s) \end{pmatrix}$$

Then

$$\langle \rho_j, \rho_k \rangle = \lambda_j, \quad j = k$$

$$= 0 \quad j = k.$$

Since

$$z_j = \langle \eta_j, f \rangle + \varepsilon_j, \quad j = 1,2,\ldots,n$$

we have

$$y_j = \langle \rho_j, f \rangle + \tilde{\varepsilon}_j$$

where

$$\begin{pmatrix} \tilde{\varepsilon}_1 \\ \vdots \\ \tilde{\varepsilon}_n \end{pmatrix} = \Gamma' \begin{pmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{pmatrix}$$

and, if the ε_i are normally distributed, the $\tilde{\varepsilon}_i$ are independent, normally distributed with mean 0 and variance σ^2. Since the experiment (1.1) provides the equivalent data y, one "knows" the inner product of f with the unit vector $\psi_i = \phi_i/\sqrt{\lambda_i}$ from the data to an accuracy of, within, say ±2 standard deviations = $2\sigma/\sqrt{\lambda_i}$. That part of f not in the span of the first r_I canonical representers is not "seen" by the experiment, even in the absence of measurement error.

4. The intrinsic rank of some examples

In these examples we suppose the t_i are equally spaced, although no doubt the results are true for $\max_i|t_{i+1}-t_i|/\min_i|t_{i+1}-t_i|$ bounded.

4.1 The first derivative, $H = H^1$

Let $H = H^1$, $H^1 = \{f: f \text{ abs. cont.}, f' \in L_2[0,1]\}$, and let

$$(Kf)(t) = \int_0^t f(s)ds,$$

thus, $\frac{d}{dt}(Kf)(t) = f(t)$. Here $\lambda_n/\lambda_1 = O(n^{-4})$. The rate $O(n^{-4})$ is obtained as follows: A reproducing kernel for H^1 is

$$R(s,t) = 1 + \min(s,t).$$

Define

$$P(s,t) = \int_0^1\int_0^1 K(s,u)R(u,v)K(t,v)dudv$$

$$= \int_0^s\int_0^t (1+\min(s,t))dsdt.$$

Then $\tilde{K}_n\tilde{K}_n^*$ is the operator of multiplication by the $n\times n$ matrix with jk^{th} entry $P(t_j,t_k)$. P is a Green's function for a 4th order linear differential operator, thus the eigenvalues of the Hilbert Schmidt operator with kernel P, are $O(n^{-4})$, i.e. inversely related to the eigenvalues of the associated differential operator. An argument in Craven and Wahba (1979), see also Wahba (1977, 1979c) indicates that the eigenvalues of the matrix obtained by discretizing P behave roughly like n times the eigenvalues of P, giving $\lambda_n/\lambda_1 = O(n^{-4})$. For a carefully developed argument which gives similar results in a related problem, see Utreras (1979).

If $n = 10^3$ then $\lambda_n/\lambda_1 \approx 10^{-12}$, and for $\delta \approx 10^{-14}$, say $\tilde{K}_n\tilde{K}_n^*$ is of full intrinsic rank. Provided that the data are not too noisy, this indicates that effective numerical differentiation is feasible if the true f is reasonably "nice".

4.2 The k^{th} derivative, $H = H^m$

Let $H = H^m$, $H^m = \{f: f, f', \ldots, f^{(m-1)}$ abs. cont., $f^{(m)} \in L_2[0,1]\}$ and let

$$(Kf)(t) = \int_0^t \frac{(t-s)^{k-1}}{(k-1)!} f(s)ds,$$

thus $\frac{\partial^k}{\partial t^k}(Kf)(t) = f(t)$. Here $\lambda_n/\lambda_1 = O(n^{-2(m+k)})$.

For example, if $k = 3$, $m = 2$, then $\lambda_n/\lambda_1 = O(10^{-10})$. If $n \sim 10^{1.4} \approx 25$, then $\lambda_n/\lambda_1 \sim 10^{-14}$ and so the intrinsic rank of this problem will be around 25. If f is a very smooth function without much structure one might expect to get a "good picture" of f with 25 pieces of information. More precisely, if f is in the span of the first 25 canonical representers and σ^2 is not too big, then a useful estimate of f might be recoverable. Otherwise it probably won't be.

This indicates, however, that accurate estimation of second derivative (k=2), with m=1 is feasible with good quality data, since in this case $\lambda_n/\lambda_1 = O(10^{-6})$ and $\tilde{K}_n\tilde{K}_n^*$ will be of full effective rank for n as large as 150.

4.3 Abel's equations

These equations are of the form

$$(Kf)(t) = \int_t^b \frac{k(t,s)}{(s-t)^\alpha} f(s)ds$$

where $k(t,s)$ is continuous on $0 \leq s \leq 1$ and $0 < \alpha < 1$. They behave like the equations in 4.2 with $k = 1 - \alpha$, and so they are of higher intrinsic rank than comparable problems involving numerical differentiation. If $H = H^m$, then $\lambda_n/\lambda_1 = O(n^{-2(m+1-\alpha)})$.

4.4 Fujita's equation and other severely ill posed problems

Fujita's equation relates centrifuge data to particle mass distribution. See Gehatia and Wiff (1970).

$$(Kf)(t) = \int_0^{s_{max}} \frac{\vartheta e^{-\vartheta st}}{1-e^{-\vartheta s}} f(s)ds \quad t\varepsilon[0,t_{max}].$$

With $\vartheta = 4.25$ and realistic values of s_{max} and t_{max} we found this innocuous looking equation to be severely ill posed. With $n = 40$ equally spaced data points, and $H = H^1$, we computed the eigenvalues $\lambda_1,\ldots,\lambda_{41}$. They turned out to look roughly as in the following table

ν	λ_ν	ν	λ_ν
1	1	6-24	10^{-14} to 10^{-15}
2	$10^{-3.5}$	25-41	-10^{-15} to -10^{-14}
3	10^{-7}		
4	$10^{-10.5}$		
5	10^{-14}		

We concluded that eigenvalues 5 or 6 through 41 were "machine 0". The intrinsic rank of this problem is between 4 and 5.

The GCV estimate of the optimal λ (the GCV estimate is defined in the next section) was around 10^{-11} and was a very good estimate of the optimal λ as measured by how close it came to minimizing

$$T_D(\lambda) = \frac{1}{n} \sum_{i=1}^{40} (f_{n,\lambda}(\tfrac{i}{41}t_{max}) - f(\tfrac{i}{41}t_{max}))^2$$

in an experiment with synthetic data where f was known. The estimate $f_{n,\lambda}$ may be written in terms of the canonical data and canonical representers of Section 3 as

$$f_{n,\lambda} = \sum_{i=1}^{n} \frac{y_i}{\lambda_i+\lambda} \rho_i .$$

Note that a λ of 10^{-11} is completely negligible compared to eigenvalues 1-3, and completely swamps eigenvalues 5-41. We succeeded in obtaining excellent solutions in some examples and nonsense results in others. See Wahba (1979c). We came to the conclusion that the excellent solutions occurred when f was effectively in the span of the first 4 canonical representers and the lousy results occurred when it was not.

Numerical inversion of the Laplace transform can be expected to be similarly nasty. The problem of inversion of radiance measurements (z) to obtain temperature profiles (f) from satellite radiance measurements in the NIMBUS 6 satellite and others also appears to be severely ill posed. See Smith and Wolfe (1976), Fritz et al (1972).

5. Solution methods for mildly ill posed problems

5.1 The method of generalized cross validation (GCV) for choosing λ

We review this method since it plays a role in the remainder of the paper. The theory has been developed in Wahba (1977), Craven and Wahba (1979) and Golub, Heath and Wahba (1979). We will refer to these last two as CW and GHW respectively. Numerical results concerning the method are given or mentioned in CW, GHW, Utreras (1979), Merz (1979), Welch (1979), Bjorck and Elden (1979), Stutzle (1977), Colli Franzone et al (1979).

The idea is as follows: Let $f_{n,\lambda}^{[k]}$ be the minimizer of

$$\frac{1}{n}\sum_{\substack{i=1\\ i\neq k}}^{n}((Kf)(t_i)-z_i)^2 + \lambda\|f\|^2,$$

where $\|\cdot\|$ may be a norm or seminorm in H. If λ is a good choice, then $(Kf_{n,\lambda}^{(k]})(t_k)-z_k$, should, on average be small. This is measured by the ordinary cross validation function $V_0(\lambda)$ given by

$$V_0(\lambda) = \frac{1}{n}\sum_{k=1}^{n}[(Kf_{n,\lambda}^{[k]})(t_k)-z_k]^2.$$

The following identity is proved in CW and GHW:

$$V_0(\lambda) \equiv \frac{1}{n}\sum_{i=1}^{n}\frac{[(Kf_{n,\lambda})(t_k)-z_k]^2}{(1-a_{kk}(\lambda))^2}$$

where $f_{n,\lambda}$ is the minimizer of

$$\frac{1}{n}\sum_{i=1}^{n}((Kf)(t_i)-z_i)^2 + \lambda\|f\|^2$$

and $a_{kk}(\lambda)$ is the kk^{th} entry of the $n\times n$ matrix satisfying

$$\begin{pmatrix} (Kf_{n,\lambda})(t_1) \\ \vdots \\ (Kf_{n,\lambda})(t_n) \end{pmatrix} = A(\lambda)z.$$

It is shown in CW and GHW that, from the point of view of minimizing predictive mean square error (defined later), $V_0(\lambda)$ should be replaced by the generalized cross validation function (GCVF) $V(\lambda)$ given by

$$V(\lambda) = \frac{1}{n}\sum_{i=1}^{n}\frac{[(Kf_{n,\lambda})(t_k)-z_k]^2}{(1-a_{kk}(\lambda))^2}\omega_k^2(\lambda) \qquad (5.1.1)$$

where

$$\omega_k(\lambda) = (1-a_{kk}(\lambda))/(1-\frac{1}{n}\sum_{j=1}^{n}a_{jj}(\lambda)).$$

Note that $a_{kk}(\lambda) = \frac{\partial}{\partial z_k}(Kf_{n,\lambda})(t_k)$, and that if all the $a_{kk}(\lambda)$ are equal, then $V(\lambda) = V_0(\lambda)$. Collapsing (5.1.1) results in

$$V(\lambda) = \frac{\frac{1}{n}||(I-A(\lambda))z||^2}{(\frac{1}{n}Tr(I-A(\lambda)))^2}. \qquad (5.1.2)$$

The GCV estimate $\hat{\lambda}$ of λ is the minimizer of (5.1.2). It is shown in CW and GHW that the minimizer of $V(\lambda)$ estimates the minimizer of the predictive mean square error $T(\lambda)$,

$$T(\lambda) = \frac{1}{n}\sum_{i=1}^{n}((Kf_{n,\lambda})(t_i)-(Kf)(t_i))^2$$

where f is the true answer in the model (1.1). There are other, possibly more desirable optimality criteria for λ, for example the minimization of

$$T_D(\lambda) = \int_0^1 (f_{n,\lambda}(t)-f(t))^2dt,$$

see also Nashed (1979b). One can obtain estimates for λ from the data

which in theory (approximately) minimize T_D. Doing this in itself is however, an ill posed problem. In our numerical experiments with synthetic data we have generally found that the minimizers of $T_D(\lambda)$ and $T(\lambda)$ tend to be close, and $\hat{\lambda}$, the minimizer of $V(\lambda)$, is generally a good estimate of the minimizer of $T(\lambda)$. For this reason we have not seriously attempted to modify the optimality criteria. In a synthetic experiment, the inefficiency of $\hat{\lambda}$ can be measured by

$$T(\hat{\lambda})/\min_{\lambda} T(\lambda) \text{ (or } T_D(\hat{\lambda})/\min_{\lambda} T_D(\lambda)).$$

5.2 Estimation of the first derivative

Here the model is

$$z_i = g(t_i) + \varepsilon_i,\ i = 1,2,\ldots,n \tag{5.2.1}$$

where the ε_i are as before and $g \in W^2$. It is desired to estimate g'. We let $g_{n,\lambda}$ be the minimizer in W^2 of

$$\frac{1}{n}\sum_{i=1}^{n}(g(t_i)-z_i)^2 + \lambda\int_0^1 (g''(u))^2 du \tag{5.2.2}$$

and estimate g' by $g_{n,\hat{\lambda}}'$, where $\hat{\lambda}$ is the minimizer of $V(\lambda)$ of (5.1.2). $g_{n,\lambda}$ is the cubic polynomial smoothing spline discussed in Reinsch (1967) and is differentiated analytically. Successful numerical results appear in CW, Merz (1978), Utreras (1979), and elsewhere.

Transportable code is available from Merz (1978), Utreras (1979) and Fleisher (1979). Our experience with the method indicates that it will do well for $n \geq 20$ or so, whenever g is "smooth", there are at least 7 or 8 data points per local maximum in g' and when σ is of the order of a fraction of a percent to several percent of the range of g.

5.3 Estimation of the second derivative. Numerical results

If g in (5.2.1) has a smooth second derivative, it can be estimated by differentiating $g_{n,\hat{\lambda}}$ twice. This should give good results in the interior of [0,1], however $g''_{n,\lambda}(0) = g''_{n,\lambda}(1) = 0$, for any λ, so that one cannot estimate g"(t) for t in a small neighborhood of 0 or 1 unless g"(0) = g"(1) = 0. This problem at the boundary can be eliminated by using quintic splines, that is, by replacing $\int_0^1 (g''(u))^2 du$ by $\int_0^1 (g'''(u))^2 du$ in (5.2.2). To my knowledge a quintic spline using GCV has not been implemented, but it could be done in a relatively straightforward manner by specializing the multidimensional results for general m in Wahba (1979a) and Wahba and Wendelberger (1979).

A Monte Carlo example of the estimation of second derivative of a periodic function in the presence of noisy data appears in Wahba (1979c), and we reproduce the example. The results were fairly typical of a large number of similar unpublished examples with high quality (Monte Carlo) data. In this example

$$g(t) = \int_0^1 K(t,s)f(s)ds$$

with

$$K(t,s) = \frac{1}{2}\{|t-s|^2 - |t-s| + \frac{1}{6}\}.$$

K(t,s) is a Green's function for the second derivative operator such that, if g = Kf, then g is the solution to g" = f, $\int_0^1 g(u)du = 0$, g(0) = g(1) = 0. The solid line in Figure 1a is g and the cross marks are the data $z_i = g(t_i) + \varepsilon_i$ where the ε_i were simulated normally distributed errors, with variance σ^2.

z was about 1/300 of the range of g. f is estimated as $f_{n,\lambda}$, the minimizer of

$$\frac{1}{n}\sum_{i=1}^{n}((Kf)(t_i)-z_i)^2 + \lambda\int_0^1 (f'(u))^2du$$

in the subspace of H^1 satisfying the (periodic) conditions $\int_0^1 f(u)du = 0$, $f(0) = f(1)$. The true f also satisfied these conditions. λ was chosen to minimize $V(\lambda)$. The calculation is that suggested in Wahba (1977), where the fact that $||\cdot||$ is a norm on the periodic functions considerably simplified the expressions. $V(\lambda)$ is plotted in 1b along with the mean square errors $T(\lambda)$ and $T_D(\lambda)$ defined by

$$T(\lambda) = \frac{1}{n}\sum_{i=1}^{n}((Kf_{n,\lambda})(t_i) - (Kf)(t_i))^2$$

and

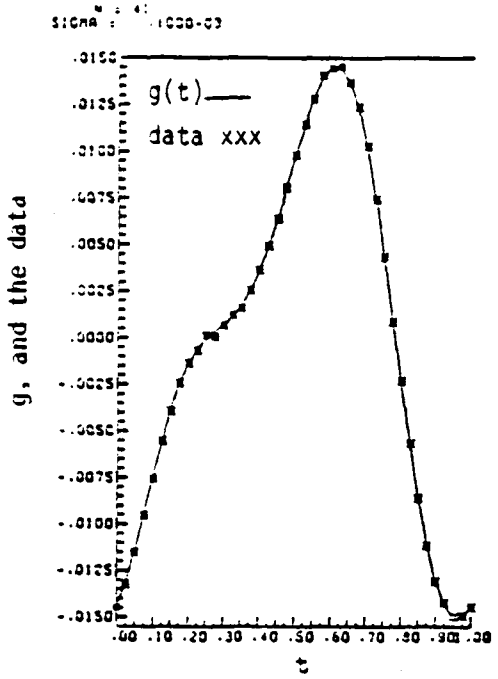
$$T_D(\lambda) = \frac{1}{n}\sum_{i=1}^{n}(f_{n,\lambda}(t_i)-f(t_i))^2.$$

It can be seen that the minimizer of $V(\lambda)$ is a good estimate of the minimizer of both $T(\lambda)$ and $T_D(\lambda)$. The theory in CW and GHW says that $V(\lambda)$ should "track" $T(\lambda)$ and one can see that this does in fact happen. Figure 1c compares the true and estimated second derivative. It can be seen that the results are very good.

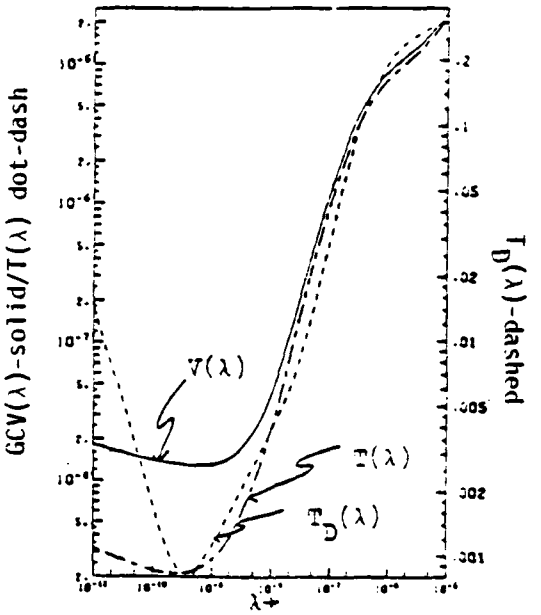
Interest in estimating the second derivative was motivated by the following problem. The Lamm equation

$$\frac{\partial c}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}(rD\frac{\partial c}{\partial r} - s\omega^2r^2c) \qquad (5.3.1)$$

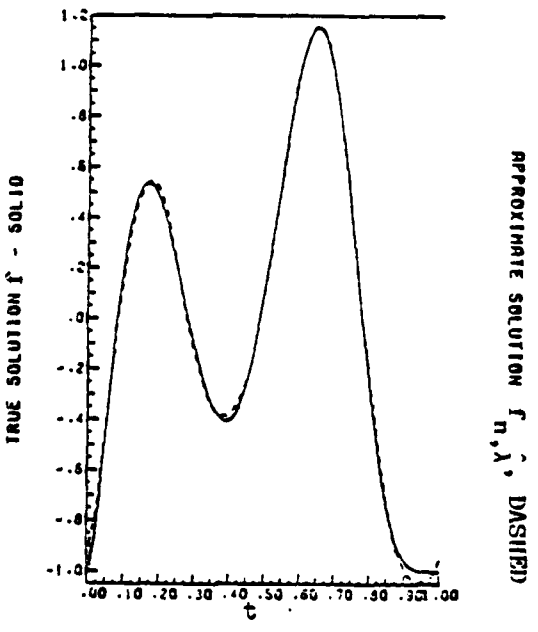
where $c = c(r,t)$ is the solute concentration, D the diffusion coefficient, s the sedimentation coefficient, and ω the angular velocity, describes the behavior of solution concentration in an ultracentrifuge. r is radial distance from the centrifugal axis and t is time. See Dishon, Weiss and



(a) The true g and the data



(b) The GCV function $V(\lambda)$ and the mean square errors $T(\lambda)$ and $T_D(\lambda)$ in $Kf_{n,\lambda}$ and $f_{n,\lambda}$.



(c) The true and estimated second derivative.

Figure 1. Estimation of Second Derivative

Yphatis (1966). ω is known. $c(r,t)$ is measured for a finely spaced set of r's at a number of values of t. From this data, it is desired to estimate D and s. The Lamm equation can be rewritten as

$$c(r,t) = \vartheta_1[\frac{1}{r}\frac{\partial c}{\partial r} + \frac{\partial^2 c}{\partial r^2}] + \vartheta_2 \frac{\partial c}{\partial t}$$

where

$$\vartheta_1 = \frac{D}{2s\omega^2} \ , \ \vartheta_2 = \frac{1}{2s\omega^2} \ .$$

If $\frac{\partial c}{\partial r}$, $\frac{\partial^2 c}{\partial r^2}$ and $\frac{\partial c}{\partial t}$ can be estimated from the data, then ϑ_1 and ϑ_2 can be estimated using regression techniques. The idea is to take an r slice of the data for fixed t and use the smoothing spline technique with GCV to estimate $\frac{\partial c}{\partial r}$ and $\frac{\partial^2 c}{\partial r^2}$, similarly with t slices of the data. Centrifuge data is frequently of the quantity and quality similar to this example, and it appears that estimating ϑ_1 and ϑ_2 is quite feasible, assuming that the model 5.3.1 reasonably represents reality and sufficient data is available.

5.4 Abel's equations

These equations have been studied by Anderssen (1976), Anderssen and de Hoog (1979), Anderssen and Jakeman (1975) and Jakeman and Anderssen (1975a,b). They have provided solution methods and a number of numerical results. Anderssen and de Hoog (1979) have called these problems "weakly ill posed". Some of these equations have inversion formulae involving the first derivative. For example (Anderssen (1976)) if

$$g(t) = 2 \int_{t}^{t_{max}} \frac{sf(s)}{(s^2-t^2)^{1/2}}\, ds \qquad (5.4.1)$$

then

$$f(s) = -\frac{1}{\pi} \int_{s}^{t_{max}} \frac{g'(t)}{(t^2-s^2)^{1/2}}\, dt. \qquad (5.4.2)$$

In addition to the spectral differentiation - product integration methods proposed by Anderssen and Jakeman (1975) the following procedure should be quite effective. If $z_i = g(t_i) + \varepsilon_i$ is observed for $i = 1,2,\ldots,n$, then g is estimated by $g_{n,\lambda}$ and g' is estimated by $g'_{n,\lambda}$ as in Section 5.2. Since $g'_{n,\lambda}$ is a polynomial of degree 2 in each interval $[t_i,t_{i+1}]$, $g'_{n,\lambda}$ can be substituted into (5.4.2) and the integration carried out analytically. This is possible using formulas 129, 136, and 153 of Pierce-Foster (1956). In some examples, g is a density and only observations $X_1,\ldots,X_n$ from this density are available. See Jakeman and Anderssen (1975b). Using a spline density estimate for g (see Wahba (1975, 1976)) would allow the analytical integration of (5.4.2). These two spline methods do not however as yet have associated with them automatic methods for choosing the optimal regularization parameter. Based on our experience with density estimates, we conjecture that the following method will be effective. Use Wahba (1978) to obtain an estimate for the density g from $X_1,\ldots,X_n$. This method has an optimal integrated mean square error procedure for choosing the smoothing parameter as part of the density estimation. The estimate so obtained is "close" to a spline. Interpolate this density estimate with a cubic spline with convenient knots, and use the spline interpolant to the density estimate in the analytical integration of (5.4.2). (This last is, of course, a form of product integration!).

Fymat and Mease (1978) have also studied first kind equations possessing inversion formulae involving the derivative of Kf.

5.5 A "general purpose" algorithm for $25 \leq n \leq 100$

In this section we elaborate on Wahba (1977) and give a "general purpose" algorithmic approach for mildly ill posed problems. (We say "general purpose" advisedly.) The upper limit on n is determined by limitations on computing the eigenvalue-eigenvector decomposition of an n×n matrix. It is assumed that the errors in the data are relatively small and random and that K is known correctly. Certain integrals below must either be known analytically or amenable to accurate quadrature.

The approach is the "Eastern" route described by Nashed (1979) in which discretization beyond that imposed by the data is done as late as possible. In the approach we take, any required numerical quadrature is isolated, and hopefully quadrature errors can be controlled so that they are negligible compared to experimental errors in the data. (This may not always be true, for example, with K such as found in scattering problems like those considered in Fymat and Mease (1978)).

The algorithm is based on the following:

Theorem: Let $H^m = \{f: f, f', \ldots, f^{(m-1)}$ abs. cont., $f^{(m)} \in L_2[0,1]\}$. Let $\omega_1, \ldots, \omega_m$ span the space of polynomials of degree m-1, and suppose the n×m matrix T with $i\nu^{th}$ entry $[T]_{i\nu}$ given by

$$[T]_{i\nu} = \int_0^1 K(t_i,s)\omega_\nu(s)ds$$

is of rank m. Then the solution to the problem: Find $f \in H^m$ to minimize

$$\frac{1}{n}\sum_{i=1}^{n}((Kf)(t_i)-z_i)^2 + \int_0^1 (f^{(m)}(s))^2 ds \qquad (5.5.1)$$

is unique and is given by

$$f_{n,\lambda}(s) = \sum_{i=1}^{n} c_i \eta_i(s) + \sum_{\nu=1}^{m} d_\nu \omega_\nu(s)$$

where

$$\eta_i(s) = \int_0^1 K(t_i,u)R(s,u)du$$

$$R(u,v) = \int_0^1 \frac{(u-x)_+^{m-1}}{(m-1)!} \frac{(v-x)_+^{m-1}}{(m-1)!} dx$$

and $c = (c_1,\ldots,c_n)'$, $d = (d_1,\ldots,d_m)'$ are determined by

$$(K_n+n\lambda I)c + Td = z$$

$$T'c = 0,$$

where K_n is the $n\times n$ matrix with jk^{th} entry

$$[K_n]_{jk} = \int_0^1\int_0^1 K(t_j,u)R(u,v)K(t_k,v)dudv.$$

A proof of this theorem may be found in Kimeldorf and Wahba (1971) Lemma 5.1 where a different but equivalent system of equations is given for c and d. See also Hilgers (1976).

We now turn to the computation of $f_{n,\hat{\lambda}}$, where $\hat{\lambda}$ is the minimizer of $V(\lambda)$. It is desirable to formulate the calculations in terms of a convenient $n\times n-m$ matrix U with the properties

$$U'U = I_{n-m\times n-m}$$

$$U'T = 0_{n-m\times n} \quad .$$

Given such a matrix, it can be shown (see Anselone and Laurent (1968)) that

$$c = U(U'K_nU+n\lambda I)^{-1}U'z$$

$$d = (T'T)^{-1}T'(z-K_nc)$$

and (Wahba (1979a))

$$I-A(\lambda) = n\lambda U(U'K_nU+n\lambda I)^{-1}U'.$$

In Wahba (1979a) and Wahba and Wendelberger (1979), we have successfully computed c,d and $V(\lambda)$ in some two dimensional spline problems which have equations of the same structure, in the following manner, using double precision EISPAC (B.T. Smith, et. al. (1976)). U is obtained with EISPACK as the matrix whose n-m columns are the n-m eigenvectors of the rank n-m projection matrix $I - T(T'T)^{-1}T'$ corresponding to the n-m unit eigenvalues. These eigenvectors are not uniquely determined, any set spanning the space perpendicular to the columns of T are allowed. Letting B be the n-m × n-m matrix $U'K_nU$, with eigenvalue decomposition $U'K_nU = \Gamma D\Gamma'$, with Γ and D again found by EISPACK, then

$$c = U\Gamma(D+n\lambda I)^{-1}\Gamma'U'z$$

and

$$V(\lambda) = \frac{\frac{1}{n}\sum_{i=1}^{n-m}\frac{(n\lambda)^2}{(d_i+n\lambda)^2}y_i^2}{(\frac{1}{n}\sum_{i=1}^{n-m}\frac{n\lambda}{d_i+n\lambda})^2}$$

where

$$y = (y_1,\ldots,y_{n-m})' = U'z$$

and $D = \mathrm{diag}(d_1,\ldots,d_{n-m})$.

For $m = 1$

$$R(u,v) = u, \; u \leq v$$
$$= v, \; u \geq v$$

and for $m = 2$

$$R(u,v) = \frac{u^2 v}{2} - \frac{u^3}{6}, \; u < v$$
$$= \frac{uv^2}{2} - \frac{v^2}{6}, \; u \geq v \quad .$$

The calculation proceeds by computing K_n by a high powered quadrature formula and $\eta_i(s)$ also by quadrature, on a fine grid in s.

In the work on second derivative and Fujita's equation noted in Sections 4.4 and 5.3, we computed K_n and the η_i by quadrature with great success in the second derivative experiments and failure with Fujita's equation. The failure was not in the determination of K_n, η_{t_i} and d_i, since in fact excellent solutions were obtained in certain "lucky" cases, see Wahba (1979c), but the general failure is explainable by the severe ill posedness, as already noted.

The numerical quadrature can be expensive, as far as computing goes, since there is a lot of it, but we were able to perform it with sufficient accuracy that quadrature error was not evident in the results. "Expensive" of course is relative, because an "expensive" $20 computer run is frequently "cheap" compared to the cost of data collection.

These computations have also been successfully carried out in a multi-dimensional smoothing context with n as large as 130. (Wahba (1979a), Wahba and Wendelberger (1979), Wendelberger (1980). In these problems K was the identity and η_i and K_n are known analytically. We found that double precision EISPACK returned the 130 eigenvalues of $I-T(T'T)^{-1}T'$,

(which are known to be 0 or 1) to seven or eight digits.

Thus, although the above procedure has not been implemented as a whole, it appears promising for medium n, mildly ill posed problems where K is such that either K_n and η_i are known analytically or computed accurately by quadrature.

5.6 Canonical form of $f_{n,\lambda}$ using the seminorm $(\int_0^1 (f^{(m)}(u))^2 du)^{1/2}$. Choice of m.

The solution $f_{n,\lambda}$ to the minimization problem of 5.5.1 can be written in the form

$$f_{n,\lambda} = (\omega_1,\ldots,\omega_m)(T'(K_n+n\lambda I)^{-1}T)^{-1}T'(K_n+n\lambda I)^{-1}z + \sum_{i=1}^{n-m} \frac{y_i}{d_i+n\lambda}\phi_i$$

where

$$y = (y_1,\ldots,y_{n-m}) = \Gamma'U'z$$

and

$$(\phi_1,\ldots,\phi_{n-m})' = \Gamma'U'(\eta_1,\ldots,\eta_n).$$

and Γ,U and $D = \mathrm{diag}\{d_i\}$ are as in Section 5.5. (Note that while U is not uniquely determined, $\Gamma'U'$ is (if the d_i are distinct). Here the canonical representers are $\omega_1,\ldots,\omega_m$ and $(\phi_1,\ldots,\phi_{n-m})$. The intrinsic rank r_I of the experiment is m plus the intrinsic rank of D. Note that as $\lambda \to \infty$ the solution tends to

$$f_{n,\infty} = (\omega_1,\ldots,\omega_m)(T'T)^{-1}T'z,$$

the least squares regression of the data onto the span of the polynomials of degree m-1 or less.

In the above expressions dependence of T, K_n, U, Σ, and $\{\phi\}$ on m has been suppressed. As m increases, the number of "special" functions $\omega_1,\ldots,\omega_m$ increases while the d_i will go to 0 faster. It is "customary" to use m=2, however, a choice between competing m's can be made by comparing $\inf_\lambda V_m(\lambda)$, for the different m's. This is done in Wahba and Wendelberger (1979), see also Gamber (1979).

5.7 A "general purpose" algorithm for larger n. Regularization with a B-spline basis

We now continue with the type of problem considered in 5.5 where n is too large for the convenient solution of an n×n eigenvalue problem. Locker and Prenter (1978a,b) have suggested solving regularization problems in N dimensional subspaces of H^m spanned by splines, and have given some convergence theorems. See also Klein (1979). We will take the suggestion and combine it with GCV for choosing λ to provide a "general purpose" algorithm for large n. The upper limit on n will no doubt be determined by storage requirements in storing N×n arrays.

We seek the minimizer of

$$\frac{1}{n}\sum_{i=1}^{n}((Kf)(t_i)-z_i)^2+\lambda\int_0^1(f^{(m)}(u))^2du$$

in H_N^m, the subspace of H^m spanned by spline functions, which are piecewise polynomials of degree 2m-1 in each interval $[\frac{i}{N'},\frac{i+1}{N'}]$, i = 0,1,...,N'-1, joined together so as to have 2m-2 continuous derivatives. It is well known (Curry and Schoenberg (1966)), de Boor(1978) that this subspace is of dimension N=N'+2m-1, and it follows from the results of Curry and Schoenberg that it is spanned by the B-splines $B_j(t)$, j = 1,2,...,N, where,

for $t\in[0,1]$ the B_j are defined by

$$B_j(t) = B_{2m}(t+\frac{2m-j}{N'}),\ j = 1,2,\ldots,N$$

$$B_{2m}(t) = -\frac{1}{(\nu N')^{2m-1}}B(N't)$$

$$B(t) = \frac{1}{(2m-1)!}\sum_{j=0}^{2m-1}(-)^j\binom{2m}{j}(t-i)_+^{2m-1},\ t\ [0,2m]$$

$$= 0 \quad \text{otherwise}$$

where $(x)_+ = x,\ x \geq 0,\ = 0$ otherwise.

Figure 2 shows $B_j(t)$ for $m = 2$ and $j = 1,2,3,4,N-2,N-1,N$. B-spline bases of degree $2m-1$ are well known to have good approximation properties in H^m.

Given

$$f = \sum_{j=1}^{N} c_j\, B_j(t)$$

one seeks $c = (c_1,\ldots,c_n)'$ to minimize

$$\frac{1}{n}\sum((Kf)(t_i)-z_i)^2 + \lambda\int_0^1(f^{(m)}(t))^2dt$$

$$= \frac{1}{n}\sum_{i=1}^{n}(\sum_{j=1}^{N}c_j(KB_j)(t_i)-z_i)^2 + \lambda\sum_{j,k=1}^{N}c_jc_k\int_0^1 B_j^{(m)}(t)B_k^{(m)}(t)dt.$$

Let X be the $n\times N$ matrix with ij^{th} entry

$$(KB_j)(t_i) = \int_0^1 K(t_i,s)B_j(s)ds$$

and let $\sum$ be the $N\times N$ matrix with jk^{th} entry

$$\sigma_{jk} = \int_0^1 B_j^{(m)}(s)B_k^{(m)}(s)ds.$$

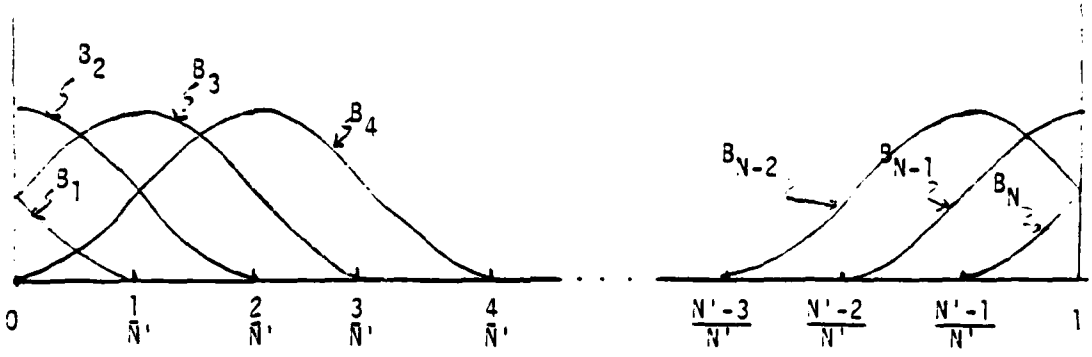


Figure 2. $B_j(t)$, for $m = 2$

The σ_{jk} for m = 2 are given in Table 1. It may be necessary to obtain the entries of X by a high-quality quadrature routine. We must find c to minimize

$$\frac{1}{n}||z - Xc||^2 + \lambda c'\Sigma c.$$

This may be done as follows:

We first note Σ is of rank N - m. This follows since the $B_1,\ldots,B_N$ are linearly independent in H^m, however $1,t,\ldots,t^{m-1}$ are in span $\{B_j\}_{j=1}^N$ so that $c'\Sigma c = 0$ if $\sum_{j=1}^N c_j B_j(t)$ is a polynomial of degree m-1 or less.

We next decompose c into a component in the null space of Σ and a component in the null space perpendicular of Σ as follows. Letting

$$\Sigma = \Gamma S \Gamma'$$

where Γ is the N×N-m matrix whose columns are the non zero eigenvectors of Σ and S the N-m×N-m matrix of non zero eigenvalues of Σ, and Δ the N×m matrix whose columns are the zero eigenvectors of Σ, then c has a unique representation as

$$c = \Gamma S^{-1/2}\gamma + \Delta d \tag{5.7.1}$$

for some $\gamma = (\gamma_1,\ldots,\gamma_{N-m})'$, $d = (d_1,\ldots,d_m)'$.

Letting

$$Y = X\Gamma S^{-1/2} \tag{5.7.2}$$

$$T = X\Delta \tag{5.7.3}$$

and assuming that T is of rank m, we have

$$Xc = Y\gamma + Td \tag{5.7.4}$$

j \ k	1	2	3	4	5	6	.	.	.	N-3	N-2	N-1	N
1	2	-3	0	1	0								
2	-3	8	-6	0	1	0							
3	0	-6	14	-9	0	1	0						
4	1	0	-9	16	-9	0	1	0					
5	0	1	0	-9	16	-9	0	⋱	⋱				
6		0	1	0	-9	16	⋱	⋱					
.			0	1	0	⋱	⋱				⋱		
.				0	⋱	⋱				⋱	⋱	0	
.					⋱				⋱	⋱	0	1	0
N-3								⋱	⋱	16	-9	0	1
N-2							⋱	⋱	0	-9	14	-6	0
N-1								0	1	0	-6	8	-3
N									0	1	0	-3	2

Table 1

$6\sigma_{jk}$, m = 2

To get $\int_0^1 B_j''(s)B_k''(s)$, divide Table entry by 6.

and γ and d are obtained by minimizing

$$\sum_{i=1}^{n}((Kf)(t_i)-z_i)^2 + n\lambda\int_0^1 (f^{(m)}(u))^2du \equiv ||z-Y\gamma-Td||^2 + n\lambda\gamma'\gamma.$$

Differentiating with respect to γ and d and setting the result equal to 0 gives the following equations for γ and d:

$$(Y'Y+n\lambda I)\gamma + Y'Td = Y'z \tag{5.7.5}$$

$$d = (T'T)^{-1}T'(z-Y\gamma). \tag{5.7.6}$$

Defining

$$P = T(T'T)^{-1}T'$$

$$W = (I-P)Y$$

and substituting (5.7.6) into (5.7.5) gives

$$\gamma = (W'W+n\lambda I)^{-1}W'z. \tag{5.7.7}$$

Let

$$W'W = VDV'$$

where V is an N-m×N-m orthogonal matrix and D is diagonal. Then

$$\gamma = V(D+n\lambda I)^{-1}V'W'z \tag{5.7.8}$$

and c is obtained by substituting (5.7.8) and (5.7.6) into (5.7.1).
To obtain $V(\lambda)$ we note that

$$\begin{aligned}(I-A(\lambda))z = z - Xc &= z - (Y\gamma+Td) = z - (Y\gamma+P(z-Y\gamma)) \\ &= (I-P)z - (I-P)Y\gamma \\ &= (I-P)z-W(W'W+n\lambda I)^{-1}W'z.\end{aligned}$$

Thus

$$(I-A) = (I-P) - W(W'W+n\lambda I)^{-1}W'$$

and, letting $d_1,\ldots,d_{N-m}$ be the diagonal entries of D, gives

$$\mathrm{Tr}(I-A) = n - m - \sum_{j=1}^{N-m} \frac{d_j}{d_j+n\lambda}$$

$$= n - N + \sum_{j=1}^{N-m} \frac{n\lambda}{d_j+n\lambda} \quad .$$

The intrinsic rank of this experiment is m + the intrinsic rank of D.

Finally,

$$||(I-A)z||^2 = ||(I-P)z||^2 - 2z'W(W'W+n\lambda I)^{-1}W'z$$

$$+ z'W(W'W+n\lambda I)^{-1}W'W(W'W+n\lambda I)^{-1}W'z$$

$$= ||(I-P)z||^2 - \sum_{j=1}^{N-m} \frac{(2n\lambda+d_j)}{(n\lambda+d_j)^2} x_j^2$$

where $x = (x_1,\ldots,x_{N-m})' = V'W'z$. Thus

$$V(\lambda) = \frac{\{||(I-P)z||^2 - \sum_{j=1}^{N-m} \frac{(2n\lambda+d_j)}{(n\lambda+d_j)^2} x_j^2}{(n-N+\sum_{j=1}^{N-m} \frac{n\lambda}{(n\lambda+d_j)})^2} \quad .$$

The calculations are summarized in Table 2.

Table 2

Summary of Calculations for
Regularization and GCV with a B-spline basis

$$\Sigma = \Gamma S \Gamma' \qquad *$$

$$Y = X\Gamma S^{-1/2}$$

Let Δ satisfy $\Gamma'\Delta = 0_{N-m\times m}$ *

$$T = X\Delta$$

$$P = T(T'T)^{-1}T'$$

$$W = (I-P)Y$$

$$WW' = VDV' \ , \ D = \mathrm{diag}(d_1,\ldots,d_{N-m}) \qquad *$$

$$\gamma = V(D+n\lambda I)^{-1}V'W'z$$

$$d = (T'T)^{-1}T'(z-Y\gamma)$$

$$c = \Gamma S^{-1/2}\gamma + \Delta d$$

$$x = V'W'z$$

$$V(\lambda) = \frac{||(I-P)z||^2 - \sum_{j=1}^{N-m} \frac{2n\lambda+d_j}{(n\lambda+d_j)^2} x_j^2}{(n-N+\sum_{j=1}^{N-m} \frac{n\lambda}{(n\lambda+d_j)})^2}$$

Note that T'T is m×m, S is well conditioned. The eigenvalue decompositions at (*) can be done in double precision EISPACK for N up to 100 or more.

6. The use of outside information. GCV in constrained regularization

Westwater (1979) and Jackson (1979) have described experiments where outside information has greatly improved the estimate of the solution. For example Westwater described how external measurement of the temperature inversion height aided in the determination of atmospheric temperature profiles.

In this section we consider first the situation when the values of one or more continuous linear functionals of f are known, either approximately or exactly.

Then we consider the situation where it is known that f is in a given closed convex set in H. If H is a reproducing kernel space then the important special case $f(t) \geq 0$, $t \in [0,1]$ is included here. Chambless (1979) has used positivity constraints in a form similar to that which we discuss here. See also Wegman (1980). Sabatier (1977) considers positivity constraints from an entirely different point of view.

A third situation arises when detailed information concerning the possible shapes of the solution is available, for example, as mentioned in Section 4.4 when libraries of temperature profiles obtained from balloon measurements are available when attempting to estimate the temperature profile from satellite radiance data (Smith and Woolf (1976)). It is possible to add various constraints, do regularization, etc. in this context but we will not discuss this situation further.

In this section we assume that n is small enough that an n×n eigenvalue problem can be solved, and we operate in the general context of Section 5.5, with some simplifications. Everything can be carried over to the B-spline basis approach in Section 5.7 but we omit the discussion.

6.1 Values of ℓ continuous linear functions are known approximately

In this section we use the notation and methods of Section 5.5. It is assumed that one observes

$$z_i = \int_0^1 K(t_i,s)f(s)ds + \varepsilon_i, \quad i = 1,2,\ldots,n \tag{6.1.1}$$

as well as

$$\tilde{y}_j = \tilde{N}_j f + \varepsilon_{n+j} \quad j = 1,2,\ldots,\ell, \tag{6.1.2}$$

where the $\tilde{N}_j$ are continuous linear functionals on H^m, and the $\varepsilon_{n+1},\ldots,\varepsilon_{n+\ell}$ are independent zero mean random variables with variance $\delta_j^2\sigma^2$, $j = 1,2,\ldots,\ell$. To assign appropriate weights to the data it is helpful to have some idea of the factor δ_j^2. Then one seeks $f_{n,\lambda}$ in H^m to minimize

$$\frac{1}{n+\ell}\left(\sum_{i=1}^{n}[(Kf)(t_i)-z_i]^2 + \sum_{j=1}^{\ell}(N_jf-y_j)^2\right) + \lambda\int_0^1 (f^{(m)}(u))^2du \tag{6.1.3}$$

where

$$N_j = \frac{1}{\delta_j}\tilde{N}_j, \quad y_j = \frac{1}{\delta_j}\tilde{y}_j .$$

The minimization problem is now formally mathematically the same as that of Section 5.5 with n replaced by $n + \ell$. It can be shown (see Kimeldorf and Wahba (1971)) that the minimizer of (6.1.3) is

$$f_{n,\lambda}(s) = \sum_{j=1}^{\ell} b_j\phi_j(s) + \sum_{i=1}^{n} c_i\eta_i(s) + \sum_{\nu=1}^{m} d_\nu\omega_\nu(s)$$

where the η_j and ω_ν are as in Section 5.5,

$$\phi_j(s) = N_jR(s,\cdot)$$

and $b = (b_1,\ldots,b_\ell)'$, c and d are given by

$$\left(\begin{array}{c|c} \frac{K_n}{L} & L \\ \hline & M \end{array} + (n+\ell)\alpha I\right)\begin{pmatrix} c \\ \hline b \end{pmatrix} + \begin{pmatrix} T \\ \hline T_1 \end{pmatrix} d = \begin{pmatrix} z \\ \hline y \end{pmatrix} \qquad (6.1.4)$$

$$(T' : T_1')\begin{pmatrix} c \\ b \end{pmatrix} = 0$$

where the $n\times\ell$, $\ell\times\ell$ and $\ell\times m$ matrices L, M and T_1 have their ij^{th} entries given by

$$[L]_{ij} = N_{j(s)}\int_0^1 K(t_i,u)R(u,s)du$$

$$[M]_{ij} = N_{i(s)}N_{j(t)}R(s,t)$$

$$[T_1]_{ij} = N_j\omega_i,$$

where $N_{j(s)}$ means the linear functional N_j applied to the argument expression considered as a function of s. The calculation proceeds exactly as in Section 5.5 upon replacing K_n and T by

$$\left(\begin{array}{c|c} \frac{K_n}{L'} & L \\ \hline & M \end{array}\right) \quad \text{and} \quad \begin{pmatrix} T \\ \hline T_1 \end{pmatrix}.$$

Note that

$$N_j f = f(s_j)$$

is a perfectly legitimate continuous linear functional in H^m (but not in L_2). If $N_j f = f(s_j)$ then

$$\rho_j(s) = R(s_j,s).$$

Frequently the values of f are known, say, at the endpoints, or other selected points and this can be an important source of information. The GCVF is computed as in Section 5.5 and now estimates λ which minimizes

$$T(\lambda) = \frac{1}{n+\ell}\{\sum_{i=1}^{n}((Kf_{n,\lambda})(t_i)-(Kf)(t_i))^2 + \sum_{j=1}^{\ell}(N_j f_{n,\lambda}-N_j f)^2\}$$

6.2 Values of ℓ continuous linear functionals are known exactly

Next, we suppose that the z_i are given by (6.1.1) but that outside information

$$y_i = N_i f, \quad i = 1,\ldots,\ell \tag{6.2.1}$$

is known exactly, or at least with an error that is negligible compared to the ε_i. We will assume here that ℓ is small enough and the N_i's are sufficiently linearly independent that explicit accurate numerical inversion of the $\ell\times\ell$ Gram matrix M appearing in (6.1.4) is possible. The estimate $f_{n,\lambda}$ of f that we seek is then the solution to the problem: Find $f\in H^m$ to minimize

$$\frac{1}{n}\sum_{i=1}^{n}((Kf)(t_i)-z_i)^2 + \lambda\int_0^1(f^{(m)}(s))^2ds$$

subject to

$$N_j f = y_j, \quad j = 1,2,\ldots,\ell\ .$$

It can be shown (see Kimeldorf and Wahba (1971)), that if T is of rank m and M is of rank ℓ, then the solution $f_{n,\lambda}$ to this minimization problem is unique and has the representation

$$f_{n,\lambda}(s) = \sum_{j=1}^{\ell}b_j\phi_j(s) + \sum_{j=1}^{n}c_j\eta_j(s) + \sum_{\nu=1}^{m}d_\nu\varepsilon_\nu(s) \tag{6.2.2}$$

where $b = (b_1,\ldots,b_\ell)'$, c and d are determined by

$$\left(\begin{array}{c|c} K_n + n\lambda I & L \\ \hline L' & M \end{array}\right)\left(\begin{array}{c} c \\ \hline b \end{array}\right) - \left(\begin{array}{c} T \\ \hline T_1 \end{array}\right) d = \left(\begin{array}{c} z \\ \hline y \end{array}\right) \qquad (6.2.3)$$

$$T'c + T_1'b = 0.$$

Appropriate methods for solving (6.2.3) in such a way that λ can be separated out to ease the calculation of $V(\lambda)$ depend on whether T_1 is of rank m, is 0, or is of rank between 1 and m. To avoid tedious details, and also to provide a more unified approach to constrained regularization which we can use in Section 6.3, we will replace the seminorm

$$[\int_0^1 (f''(u))^2 du]^{1/2}$$

on W^2 by the norm defined by

$$||f||^2 = \frac{1}{\vartheta}(f^2(0)+f^2(1)) + \int_0^1 (f''(u))^2 du \qquad (6.2.4)$$

which will simplify the arguments as well as the calculations considerably. This particular method of augmenting the seminorm by adding $\frac{1}{\vartheta}(f^2(0) + f^2(1))$ reflects a prior belief that the true f is near 0 at the boundaries, if this is not the case, then ϑ should be chosen large, or a different augmentation may be chosen. As $\vartheta \to 0$ the solution is forced to be 0 on the boundaries, and as $\vartheta \to \infty$ the solution tends to (6.2.2).

A reproducing kernel $Q(s,t)$ for H^2 with the norm (6.2.4) is given by [1]

$$Q(s,t) = \vartheta(st+(1-s)(1-t)) + \frac{1}{6}[-s^3(1-t)+st(t-1)(t-2)], \quad s < t,$$

$$= \vartheta(st+(1-s)(1-t)) + \frac{1}{6}[s^3t-3s^2t+s(2t+t^3)-t^3], \quad s>t \quad .$$

Using this r.k., one obtains the following:

Theorem: The solution $f_{n,\lambda}$ to the problem: Find $f\in H^2$ to minimize

$$\frac{1}{n}\sum_{i=1}^{n}((Kf)(t_i)-z_i)^2 + \lambda[\frac{1}{9}(f^2(0)+f^2(1))+\int_0^1(f''(u))^2du] \qquad (6.2.5)$$

subject to

$$N_jf = y_j, \qquad j = 1,2,\ldots,\lambda$$

is given by

$$f_{n,\lambda}(s) = \sum_{j=1}^{\lambda} b_j\phi_j(s) + \sum_{i=1}^{n} c_i\eta_i(s) \qquad (6.2.6)$$

where now

$$\phi_j(s) = N_{j(t)}Q(t,s)$$

$$\eta_i(s) = \int_0^1 K(t_i,u)Q(u,s)du$$

and c and b are given by

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[1] To verify that this is a r.k. for H^2 with the norm of (6.2.4) one must establish that $Q(\cdot,t)\in H^2$ and $\langle Q(\cdot,s),f\rangle = f(s)$ for any $f\in H^2$, where $\langle,\rangle$ is the inner product induced by (6.2.4). This verification is tedious but straightforward. $R(s,t)$ in preceeding sections is a reproducing kernel for a subspace of H^2 of codimension 2 (the polynomials having been subtracted out.)

$$\begin{pmatrix} K_n+n\lambda I & L \\ \hline L' & M \end{pmatrix} \begin{pmatrix} c \\ \hline b \end{pmatrix} = \begin{pmatrix} z \\ \hline y \end{pmatrix}$$

where K_n, L and M have their ij^{th} entries given by

$$[K_n]_{ij} = \int_0^1\int_0^1 K(t_i,u)Q(u,v)K(t_j,v)dudv \tag{6.2.7}$$

$$[L]_{ij} = N_{j(s)}\int_0^1 K(t_i,u)Q(s,u)du \tag{6.2.8}$$

$$[M]_{ij} = N_{i(s)}N_{j(t)}Q(s,t). \tag{6.2.9}$$

To obtain $V(\lambda)$ we shall use a different representation for f than (6.2.6). This representation and what follows is computationally useful provided λ is small and M is well conditioned. If M is not well conditioned, then some of the "exact" data is redundant and should be eliminated. We have

$$f_{n,\lambda}(s) = \sum_{i=1}^{2} \tilde{b}_i\phi_i(s) + \sum_{i=1}^{n} \tilde{c}_i\xi_i(s) \tag{6.2.10}$$

where

$$\tilde{b} = M^{-1}y,$$

the vector $\xi = (\xi_1(s),\ldots,\xi_n(s))$ is given by

$$\xi = \eta - LM^{-1}\phi$$

where $\eta = (\eta_1,\ldots,\eta_n)'$, $\phi = (\phi_1,\ldots,\phi_2)'$ and $\tilde{c}$ satisfies

$$(\tilde{K}+n\lambda I)\tilde{c} = z - LM^{-1}y$$

where

$$\tilde{K} = K_n - LM^{-1}L' .$$

To obtain $V(\lambda)$ note that

$$z - \begin{pmatrix} (Kf_{n,\lambda})(t_1) \\ \vdots \\ (Kf_{n,\lambda})(t_n) \end{pmatrix} = z - (LM^{-1}y) + \tilde{K}(\tilde{K}+n\lambda I)^{-1}(z-LM^{-1}y)$$

$$= (I-A(\lambda))(z-LM^{-1}y) \qquad (6.2.11)$$

where

$$A(\lambda) = \tilde{K}(\tilde{K}+n\lambda I)^{-1}.$$

Since $LM^{-1}y$ is known exactly, it is reasonable to view $z - LM^{-1}y$ as the "data vector". Then the GCVF is

$$V(\lambda) = \frac{\frac{1}{n}||(I-A(\lambda))(z-LM^{-1}y)||^2}{(\frac{1}{n}Tr(I-A(\lambda)))^2} . \qquad (6.2.12)$$

Letting $\tilde{K} = UDU'$ with $D = diag(\lambda_1,\ldots,\lambda_n)$ and $x = (x_1,\ldots,x_n)' = U'(z-LM^{-1}y)$ gives

$$V(\lambda) = \frac{\frac{1}{n}\sum_{i=1}^{n}(\frac{n\lambda}{d_i+n\lambda})^2 x_i^2}{(\frac{1}{n}\sum_{i=1}^{n}\frac{n\lambda}{d_i+n\lambda})^2} \qquad (6.2.13)$$

Before using this approach the experimenter should verify that errors in $LM^{-1}y$ are in fact entirely negligible compared to σ^2, and errors in computing M^{-1} are negligible. If this is the case, then the intrinsic rank of the problem is 2 + the intrinsic rank of D.

6.3 feC, a closed convex set in H

If H is an r.k.h.s. then

$$C = \{f: f(t) \geq \alpha(t),\ t\in[0,1]\} \tag{6.3.1}$$

is a closedconvex set in H for any continuous $\alpha(t)$, in particular, for $\alpha(t) \equiv 0$. More generally sets of the form

$$C = \{f: \alpha_k(t) \leq f^{(k)}(t),\ t\in[a,b]\}$$
$$C = \{f: f^{(k)}(t) \leq \beta_k(t),\ t\in[c,d]\}$$

etc. are closed and convex in $H^m[0,1]$ for $k \leq m - 1$. This type of information is frequently known a priori. For example if f is a particle size distribution then $f(t) \geq 0$.

Since

$$\frac{1}{n}\sum_{i=1}^{n}((Kf)(t_i)-z_i)^2 + \lambda||f||^2 \tag{6.3.2}$$

with $||\cdot||^2$ a norm is a strictly [2] convex functional in H, it always has a unique minimizer on any closed convext set C.

We will consider C as in (6.3.1) in some detail although much more general cases can be treated similarly.

Intuitively, if H is a space of continuously differentiable functions, the closed convex set of (6.3.1) can be replaced for practical purposes by the closed, convex set C_r,

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[2] In H^m with the seminorm $\int_0^1 (f^{(m)}(u))^2 du$ it is sufficient that the matrix T in Section 5.5 be of rank m. In what follows we are always assuming the strict convexity of (6.3.2) and the analogous expression with the k^{th} term in the sum omitted.

$$C_r = \{f: \alpha(s_j) \leq f(s_j),\ j = 1,2,\ldots,r\}$$

where $s_1, s_2, \ldots, s_r$ is a sufficiently fine mesh in $[0,1]$. For related convergence theory see Laurent and Martinet (1969), Wahba (1973).

The solution $f_{n,\lambda}$ to the problem: find $f \in H^2$ to minimize

$$\frac{1}{n}\sum_{i=1}^{n}((Kf)(t_i)-z_i)^2 + \lambda\{\frac{1}{\theta}(f^2(0)+f^2(1)) + \int_0^1 (f''(u))^2 du\} \qquad (6.3.3)$$

subject to

$$\alpha(s_j) \leq f(s_j), \quad j = 1,2,\ldots,r$$

is given by

$$f_{n,\lambda}(s) = \sum_{j=1}^{r} b_j Q(s_j,s) + \sum_{i=1}^{n} c_i \eta_i(s) \qquad (6.3.4)$$

where b anc c are solutions to the quadratic programming problem: Find b and c to minimize

$$\frac{1}{n}||Lb+K_n c-z||^2 + \lambda(b'Mb+2b'Lc+c'K_n c)$$

subject to

$$Qb + L'c \geq \alpha,$$

where $||\cdot||$ is the Euclidean norm, $\alpha = (\alpha(s_1),\ldots,\alpha(s_r))'$, K_n is given by (6.2.7) and the ij^{th} entries of L and M are given by

$$[L]_{ij} = \int_0^1 K(t_i,u)Q(u,s_j)du$$
$$[M]_{ij} = Q(s_i,s_j).$$

(See Kimeldorf and Wahba (1971)).

If n + r is under around 150 the solutions b and c to this problem can usually be obtained numerically, for fixed λ, from available library quadratic programming routines (for example, Madison Academic Computing Center (1977)).

We suggest the following procedure, provided that it is sufficient to consider fairly small r. Here λ is fixed. Solve the unconstrained problem. If the solution $f_{n,\lambda}$ satisfies all the constraints $f_{n,\lambda}(s_j) \geq \alpha(s_j)$, $j = 1,2,\ldots,r$, stop. Otherwise, find $j = j_1$ for which $f_{n,\lambda}(s_j) - \alpha(s_j)$ is most negative. Minimize (6.3.2) subject to $f(s_{j_1}) - \alpha(s_{j_1}) \geq 0$. If the solution, call it $f_{n,\lambda}^{(j_1)}$ satisfies all the constraints, stop. Otherwise find j_2 such that $f_{n,\lambda}^{(j_1)}(s_j) - \alpha(s_j)$ is most negative. Minimize (6.3.2) subject to $f(s_{j_\nu}) - \alpha(s_{j_\nu}) \geq 0$, $\nu = 1,2$. If the solution satisfies all the constraints, stop. Otherwise proceed to add one (or possibly several) of the most violated constraint(s) until a solution satisfying all the constraints is found.

A much more elegant iterative procedure, where one only has to carry along two linear combinations of active constraints, can be developed based on Laurent and Martinet (1969) (personal communication, P.J. Laurent). It is intended that this will appear separately.

If the solution to the unconstrained problem with a good choice of λ satisfies the constraints, then of course, one is finished. If it is necessary to impose constraints, then it is not necessarily true that one wants the same λ, since the imposition of constraints is in a sense a form of regularization. From this point of view, an optimal λ for a problem with active constraints is likely to be smaller. We discuss the choice of λ for constrained problems next.

6.4 Generalized cross-validation for constrained problems (GCVC)

We now discuss the establishement of a generalized cross-validation function for constrained problems (GCVFC). Theoretical results for GCVC have not been established, but we believe they can be. At the end we

discuss some possible computational strategies. In the following discussion we return to general H, where $|\!|\cdot|\!|$ may be a norm or a seminorm.

We believe the correct (first order) generalization of the GCVF is the generalized cross validation function for constrained problems (GCVFC) given by

$$V(\lambda) = \frac{\frac{1}{n}\sum_{i=1}^{n}((Kf_{n,\lambda})(t_i)-z_i)^2}{(1-\frac{1}{n}\sum_{i=1}^{n}a_{ii}(\lambda,z))^2} \tag{6.4.1}$$

where

$$a_{ii}(\lambda,z) = \frac{\partial}{\partial z_i}(Kf_{n,\lambda})(t_i)\Big|_z \tag{6.4.2}$$

and λ should be chosen by minimizing (6.4.1)

The expression for $V(\lambda)$ reduces to the GCVF in the unconstrained case. In the unconstrained case (or in the case C is a linear manifold as in Section 6.2) $(Kf_{n,\lambda})(t_k)$ is a linear function of z_k and $a_{kk}(\lambda,z)$ is the kk^{th} entry of the appropriate matrix $A(\lambda)$. It will be shown later than when C is determined by a finite number of linear inequality constraints, $a_{kk}(\lambda,z)$ is piecewise constant in z, and, as a consequence, a relatively straightforward algorithm for computing $V(\lambda)$ can be established.

Let C be any convex set in H and let $f_{n,\lambda}^{[k]}$ be the minimizer in C of

$$\frac{1}{n}\sum_{\substack{i=1\\ i\neq k}}^{n}((Kf)(t_i)-z_i)^2 + \lambda|\!|f|\!|^2, \tag{6.4.3}$$

where either $|\!|\cdot|\!|$ is a norm or (6.4.3) is strictly convex for each k. The "ordinary" cross validation function or "leaving out one" function $V^0(\lambda)$ may be simply defined as

$$V^0(\lambda) = \frac{1}{n} \sum_{k=1}^{n} (Kf_{n,\lambda}^{[k]}(t_k) - z_k)^2 \ . \qquad (6.4.4)$$

However $V^0(\lambda)$ will be prohibitive to compute in most cases, and it reduces, in the unconstrained case, to a procedure which can have inferior properties to the GCVF. See GHW, CW.

The rationale behind (6.4.1) is a consequence of the following lemma which generalizes Lemma 3.1 in CW.

Lemma: Let C be any closed convex set in H and let $f_{n,\lambda}$ and $f_{n,\lambda}^{[k]}$ be the minimizers of (6.3.2) and (6.4.3) and respectively in C. To indicate emphasis on z, write $f_{n,\lambda}(t,z) = f_{n,\lambda}(t)$. Then

$$f_{n,\lambda}(t,z+\delta) \equiv f_{n,\lambda}^{[k]}(t),$$

where $\delta = (0,\ldots,0,\delta_k,0,\ldots,0)$, δ_k is in the k^{th} position, and

$$\delta_k = (Kf_{n,\lambda}^{[k]})(t_k) - z_k \ .$$

Proof: Denote $f_{n,\lambda}^{[k]}$ by h and $Kf_{n,\lambda}^{[k]}(t_k)$ by $\hat{z}_k$. Then

$$\frac{1}{n}[\sum_{\substack{j=1 \\ j\neq k}}^{n} (Kh)(t_j)-z_j)^2 + ((Kh)(t_k)-\hat{z}_k))^2] + \lambda||h||^2$$

$$= \frac{1}{n} \sum_{\substack{j=1 \\ j\neq k}}^{n} ((Kh)(t_j)-z_j)^2 + \lambda||h||^2$$

$$< \frac{1}{n} \sum_{\substack{j=1 \\ j\neq k}}^{n} ((Kf)(t_j)-z_j)^2 + \lambda||f||^2, \text{ for any } f\in C \text{ other than } h$$

$$\leq \frac{1}{n}[\sum_{\substack{j=1 \\ j\neq k}}^{n} ((Kf)(t_j)-z_j))^2 + ((Kf)(t_k)-\hat{z}_k)^2] + \lambda||f||^2. \qquad (6.4.5)$$

Thus $h = f_{n,\lambda}^{[k]}$ is the minimizer of (6.4.5), which is also minimized uniquely by $f_{n,\lambda}(t,z+\delta)$.

It follows that

$$Kf_{n,\lambda}^{[k]}(t_k) \equiv (Kf_{n,\lambda})(t_k) + [(Kf_{n,\lambda})(t_k,z+\delta) - Kf_{n,\lambda}(t_k,z)]. \qquad (6.4.6)$$

Assuming that $(Kf_{n,\lambda})(t_k,z+\delta)$ is twice continuously differentiable in δ_k in the neighborhood of $\delta_k = 0$, expanding the second term on the right in (6.4.6) in a Taylor series in δ_k gives

$$Kf_{n,\lambda}^{[k]}(t_k) = (Kf_{n,\lambda})(t_k) + \delta_k \frac{\partial}{\partial z_k}(Kf_{n,\lambda})(t_k,z) + O(\delta_k^2)$$

$$= (Kf_{n,\lambda})(t_k) + (Kf_{n,\lambda}^{[k]}(t_k)-z_k)\cdot\frac{\partial}{\partial z_k}(Kf_{n,\lambda})(t_k,z) + O(\delta_k^2).$$

Setting $O(\delta_k^2) = 0$ some algebra results in the expression

$$Kf_{n,\lambda}^{[k]}(t_k)-z_k = \frac{(Kf_{n,\lambda})(t_k)-z_k}{(1-a_{kk}(\lambda,z))} \quad ,$$

giving a first order approximation to the ordinary cross-validation function of (6.4.4),

$$V^0(\lambda) = \frac{1}{n}\sum_{k=1}^{n}\frac{((Kf_{n,\lambda})(t_k)-z_k)^2}{(1-a_{kk}(\lambda,z))^2} \quad . \qquad (6.4.7)$$

Provided that the map $A(\lambda)\colon E_n \to E_n$ which maps $z \to ((Kf_{n,\lambda})(t_1),\ldots,(Kf_{n,\lambda})(t_n))'$ is locally nearly linear and the δ_k are small, the same reasoning which led the substitution of $V_0(\lambda)$ by $V(\lambda)$ in the unconstrained case should work here. (See Wahba (1977), CW, GHW). For that reason, and because $V(\lambda)$ is much easier to compute, we adopt it here.

We now study the behavior of $Kf_{n,\lambda}(t_k,z+\delta)$ as a function of δ_k, where $\delta = (0,\ldots,0,\delta_k,0,\ldots,0)$. Suppose $f_{n,\lambda}$ is the minimizer of (6.3.2) in C_r

and it is found that the constraints $f_{n,\lambda}(s_j) \geq \alpha(s_j)$ are active for $j = j_1,\ldots,j_\ell$. Then $f_{n,\lambda}$ is also the solution to the minimization problem: Find f to minimize (6.3.2) subject to the equality constraints

$$f(s_{j_\nu}) = (s_{j_\nu}),\ \nu = 1,2,\ldots,\ell.$$

Thus, except in the neighborhood of some critical points z wnere the constraints "just" become active, the dependence of $Kf_{n,\lambda}(t_k,z+\delta)$ on δ_k is linear, as can be seen by examining the results of Section 6.2, equation (6.2.2) where ℓ linear <u>equality</u> constraints are imposed.

The following artificial example with $H = E^n$ is illuminating. For this example z, $k = (k_1,\ldots,k_n)'$, $f = (f(1),\ldots,f(n))'$ and $\alpha = (\alpha(1),\ldots,\alpha(n))'$ are n vectors. The minimizer $f_\lambda = (f_\lambda(1),\ldots,f_\lambda(n))'$ of

$$\sum_{i=1}^{n}(k_i f(i)-z_i)^2 + \sum_{i=1}^{n} f^2(i)$$

subject to

$$f(i) \geq \alpha(i), \quad i = 1,2,\ldots,n$$

is given by

$$f_\lambda(i) = \frac{k_i}{k_i^{2}+\lambda} z_i,\ \frac{k_i}{k_i^{2}+\lambda} z_i \geq \alpha(i)$$

$$= \alpha(i)\ ,\ \frac{k_i}{k_i^{2}+\lambda} z_i \leq \alpha(i)\ .$$

Thus,

$$k_i f_\lambda(i) = \frac{k_i^2}{k_i^{2+\lambda}} z_i, \ \frac{k_i}{k_i^{2+\lambda}} z_i \geq \alpha(i)$$

$$= k_i \alpha(i) \ , \ \frac{k_i}{k_i^{2+\lambda}} z_i \leq \alpha(i) \quad .$$

Thus, for $i = 1,2,\ldots,\ell$

$$a_{ii}(\lambda,z) = \frac{d}{dz_i} k_i f_\lambda(i) = k_i^2 (k_i^{2+\lambda})^{-1}, \ \frac{k_i}{k_i^{2+\lambda}} z_i > \alpha(i)$$

$$= 0 \qquad \frac{k_i}{k_i^{2+\lambda}} z_i < \alpha(i)$$

$$\text{undefined} \qquad \frac{k_i}{k_i^{2+\lambda}} z_i = \alpha(i) \quad .$$

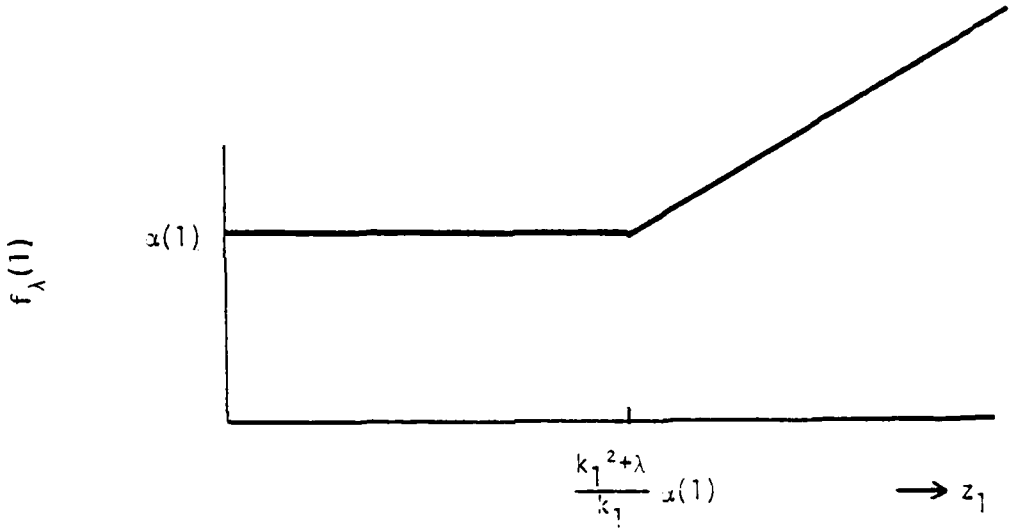
See Figure 3 for a plot of $f_\lambda(1)$ and $\frac{d}{dz_1} k_i f_\lambda(1)$ as a function of z_1.

For fixed z, the denominator $(1-\frac{1}{n} \sum_{i=1}^{n} a_{ii}(\lambda,z))^2$ in the GCVFC, can be a discontinuous function of λ as constraints become active or inactive with varying λ, that is, as λ satisfies

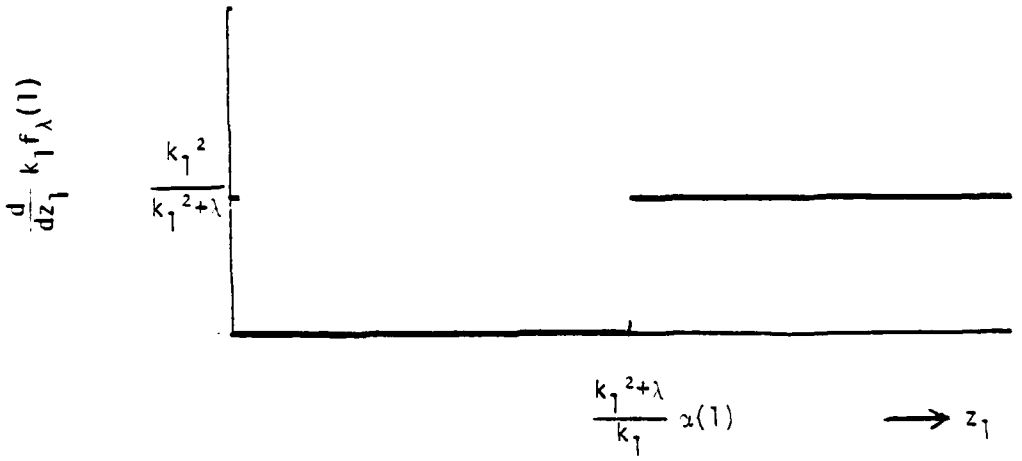
$$\frac{k_i}{k_i^{2+\lambda}} z_i = \alpha(i), \qquad i = 1,2,\ldots,\ell.$$

It can be conjectured that if n is large that this will not be a serious practical problem, but no numerical evidence is available at this time.

The GCVF of (6.4.1) for fixed λ is obtained as follows. For concreteness we suppose $H = H^2$, with the norm $\|\cdot\|$ given by (6.2.4). For given λ suppose the solution $f_{n,\lambda}$ to the constrained minimization problem with constraints $f(s_j) \geq \alpha(s_j)$, $j = 1,2,\ldots,r$ has been obtained and the ℓ



(a) $f_\lambda(1)$ as a function of z_1



(b) $\frac{d}{dz_1} k_1 f_\lambda(1)$ as a function of z_1

Figure 3

constraints corresponding to $j = j_1,\ldots,j_\ell$ have found to be active. Hopefully ℓ will not be too large. Then applying the results of Section 6.2, equations (6.2.11) and (6.2.12) give

$$\begin{pmatrix} (Kf_{n,\lambda})(t_1) \\ \vdots \\ (Kf_{n,\lambda})(t_n) \end{pmatrix} = A(\lambda)(z-LM^{-1}\alpha) + LM^{-1}\alpha$$

with $\alpha = (\alpha(j_1),\ldots,\alpha(j_\ell))'$, where

$$A(\lambda) = \tilde{K}(\tilde{K}+n\lambda I)^{-1}$$
$$\tilde{K} = K_n - LM^{-1}L'$$

where K_n is given by (6.2.7) and L and M are $n\times\ell$ and $\ell\times\ell$ matrices with entries given by

$$[L]_{i\nu} = \int_0^1 K(t_i,u)Q(u,s_{j_\nu})du \qquad i = 1,2,\ldots,n \quad \nu = 1,2,\ldots,\ell$$

and

$$[M]_{\mu\nu} = Q(s_{j_\mu},s_{j_\nu}) \qquad \mu,\nu = 1,2,\ldots,\ell \ .$$

Therefore, by (6.2.12)

$$V(\lambda) = \frac{\frac{1}{n}||(I-A(\lambda))(z-LM^{-1}\alpha)||^2}{(\frac{1}{n}Tr(I-A(\lambda)))^2} \tag{6.4.8}$$

and it can be computed as in (6.2.13), provided ℓ is not too large.

One could define the intrinsic rank of this problem (now depending on z) as was done following (6.2.13), however, the meaning is now somewhat blurred.

An outline of the numerical determination of $V(\lambda)$ follows. It is clear that there is room for the development of an efficient overall strategy.

1) Minimize $V(\lambda)$ for the unconstrained problem. If the solution to the unconstrained problem satisfies the constraints, stop. If not, let λ_0 be the minimizer of the (unconstrained) GCVF, $V(\lambda)$.
2) Solve the constrained problem with $\lambda = \lambda_0$. Determine the active constraint indices $j_1,\ldots,j_\ell$, for λ_0 and compute the GCVFC $V(\lambda_0)$ according to (6.4.8).
3) Repeat 2) with $\lambda = \lambda_1 < \lambda_0$.
4) If $V(\lambda_1) < V(\lambda_0)$, continue to decrement λ and repeat 2) until a (global!) minimum if found. If $V(\lambda_1) > V(\lambda_0)$, increment λ and repeat 2) until a minimum if found.

It is possible that the discontinuities in $V(\lambda)$ and the fact that the GCVF involves first order approximations may lead to meaningless local minima, particularly for small n. We remark that, since the set of active constraints is likely to vary slowly with λ, it is desireable to build this into the computational strategy. We have found it convenient to work in units of log λ.

6.5 Other generalizations of the GCVFC

The definition of the GCVFC extends to other problems where $(Kf_{n,\lambda})(t_k)$ is not linear in the data.

There has been recent interest in robust smoothing, which is appropriate if the errors cannot be considered to have normal distributions, but may have outliers. For example, a robust smoothing spline is defined as the solution to: Find $f \in H^m$ to minimize

$$\frac{1}{n}\sum_{i=1}^{n}\rho(f(t_i)-z_i) + \lambda\int_0^1 (f^{(m)}(u))^2 du \qquad (6.5.1)$$

where $\rho(\cdot)$ is a suitably chosen convex functional. Once can define the GCVFN (Generalized cross-validation function for non linear problems) exactly as in (6.4.7), or as

$$V(\lambda) = \frac{\frac{1}{n}\sum\rho((Kf_{n,\lambda})(t_i)-z_i)}{(1-\frac{1}{n}\sum_{i=1}^{n}a_{ii}(\lambda,z))^2}$$

where $a_{ii}(\lambda,z)$ is as in (6.4.1). See Huber (1979), Lenth (1979). When iterative methods are used to minimize (6.5.1) $A(\lambda,z)$ may be available at the last step of the iteration. The definition (6.4.1) of $V(\lambda)$ is likely to be useful in some cases where K is a (mildly) nonlinear operator, but the state of the art of nonlinear ill posed problems appears not very advanced at this time.

7. Checking the model

With the advent of sophisticated techniques for recovering f from z, accurate specification of the "model", i.e. of K becomes increasingly more important. Frequently K is established from physical principles where simplifications, approximations and possibly erroneous assumptions have been made.

In the past it has been commonplace to blame an inability to recover a reasonable f from z on the failure of the mathematical techniques used. With better techniques this "excuse" is no longer available.

Merz (1979) and Colli Franzone et al (1979) both discovered serious inadequacies in their model after satisfactorily testing the validity of their regularization programs on simulated data. We feel this testing procedure is an obvious and important step in the analysis of data from any experiment. The experimenter should be able to construct one or several test f's that could reasonably represent the major features of f's that might in fact be present. One then simulates "data" by computing $(Kf)(t_j)$ using the K that will be used in the numerical inversion formula, and simulating measurement or instrument errors in a realistic manner by Monte Carlo methods. One then applies the numerical algorithm to the simulated data and determines how well the (known) f is recovered. Aside from easing the (non trivial!) task of the debugging of the computer program this gives the experimenter a "feel" for how well f can be recovered from the experiment assuming that the model K is accurate. At this point inadequacies in the number and placement of $t_1,\ldots,t_n$ can sometimes be identified.

We always print out the eigenvalues d_i, from this the intrinsic rank r_I can be determined by inspection. In problem cases, it is also a useful

diagnostic tool to print out the canonical representers which are associated with the largest eigenvalues. Chambless (1979) in a regularization method involving the "Western" route, or discretization first was able to explain poor performance of a certain quadrature rule compared to another, by comparing the associated canonical representers. Once this testing with a "mathematical" K and synthetic data has been successfully carried out it is very desirable to run an experiment on the real apparatus with known f. This option is not always available, but if it is, it can be very valuable, because if f has been successfully recovered in a synthetic experiment and the same f cannot be recovered from "real" data, the source of the problem is pinpointed in an inadequate representation of K or inadequate understanding of the experimental error.

It would be nice to have a "goodness-of-fit" test for the model K (more precisely, for $\tilde{K}_n$). Goodness-of-fit tests of the classical statistical form cannot be rigorously derived in the context of most ill posed problems because there are no degrees of freedom for error. However, we will describe a loose approximation to a goodness-of-fit test, based on an analogy with regression.

To describe the regression situation, let K be an n×p matrix, $p < n$, of rank p, and f be a p vector. The classical regression model is

$$z = Kf + \varepsilon.$$

ε is as before.

The Gauss-Markov estimate of f is $\hat{f}$,

$$\hat{f} = (K'K)^{-1}K'z.$$

The data vector z is partitioned into "signal" $K\hat{f}$

$$K\hat{f} = Az, \quad A = K(K'K)^{-1}K'$$

and noise $\hat{\varepsilon}$,

$$\hat{\varepsilon} = (I-A)z.$$

If K is the correct model, then $\hat{\sigma}^2$ given by

$$\hat{\sigma}^2 = \frac{||(I-A)z||^2}{n-p} = \frac{||(I-A)z||^2}{Tr(I-A)}$$

is an estimate of σ^2 and $\chi^2 = (n-p)\hat{\sigma}^2/\sigma^2$ has the chi-squared distribution with n-p degrees of freedom. Assuming σ^2 is known, then χ^2 can be compared to the upper 99% point, say of the χ^2 distribution with n-p degrees of freedom. Since $(I-A)K \equiv 0$, $(I-A)z = (I-A)\varepsilon$ assuming K is the correct model, and if the true model is actually K* with $(I-A)K^* \neq 0$, then $\hat{\sigma}^2/\sigma^2$ will tend to be too large.

By analogy in the regularization case (and reverting to the notation of earlier sections) the data vector z is partitioned into signal

$$((Kf_{n,\hat{\lambda}})(t_1),\ldots,(Kf_{n,\hat{\lambda}})(t_n))' = A(\hat{\lambda})z,$$

and noise

$$\hat{\varepsilon} = (I-A(\hat{\lambda}))z,$$

where $\hat{\lambda}$ is the minimizer of $V(\lambda)$. Then

$$\hat{\sigma}^2 = \frac{||(I-A(\hat{\lambda}))z||^2}{Tr(I-A(\hat{\lambda}))}$$

is an estimate for σ^2. Letting $\tilde{K}_n: H \to E_n$ be the operator defined in Section 2, it can be seen that some "signal" creeps into $\hat{\varepsilon}$, since $(I-A(\hat{\lambda}))\tilde{K}_n f \neq 0$

even if $\tilde{K}_n$ is the correct model. However, $||(I-A(\hat{\lambda}))\tilde{K}_n f||$ should be small compared to $||(I-A(\hat{\lambda}))\varepsilon||^2$ for large n. Usually the experimenter has some idea about the size of σ^2. Then $\chi^2 \approx Tr(I-A(\hat{\lambda}))\hat{\sigma}^2/\sigma^2$ can be compared to the upper tail of a χ^2 distribution with approximately $Tr(I-A(\hat{\lambda}))$ degrees of freedom. If $\hat{\sigma}^2/\sigma^2$ is very much too large this may be some evidence that the $\tilde{K}_n$ is inaccurate. If $\hat{\sigma}^2/\sigma^2$ is too small, the GCVF may be erroneously attempting to interpolate the data. Results of any such tests should be taken with a grain of salt until the properties of the test have been verified on synthetic data. We also remind the reader that sparse poor quality data will support or fail to reject a bigger class of models than plentiful, good data.

3. Regularization in extremely large problems. The Landweber iteration and GCV

In computerized tomography (CT) and related indirect sensing problems the number of data points can be in the many thousands. The computerized X-Ray tomography problem is actually very mildly ill posed, and there exist inversion formulae similar to Abel inversion formulae in two dimensions. See Herman and Naparstek (1977). It is fortunate that the problem is only mildly ill posed, since this allows the reconstruction of complex images. The 1979 Nobel Prize in Physiology or Medicine was awarded for work in CT, see deChiro and Brooks (1979).

Most recent computerized CT systems use transform methods and the amount of regularization is chosen at the design stage by trial and error with real or "phantom" data. This choice typically involves both subjective and objective evaluation of the resulting picture. (Artzy, Elfving and Herman (1979), Naparstek, personal communication).

The first commercial machines discretized the problem at the start and solved the resultant large linear system approximately by Kaczmarz iteration, also known as "ART". In this Section we discuss only the Landweber iteration although it appears that similar results can be obtained for other iterative methods. It has been observed by Miller (1974), Strand (1976), Fleming (1977), Bjorck and Elden (1979) that the number of iterations in a Landweber iteration for solving a linear system plays the role of a regularization parameter. We will elaborate on some of the ideas in those papers and show how GCV can be used to choose the number of iterations and other regularization parameters in such a technique without actually solving an eigenvalue problem.

In this section, Nashed's "Western route" has been taken and the operator K is assumed to have been discretized to an $n \times r$ matrix, say, where $r<n$, and n and r are very large. K is considered as an operator from E^r

to E^n, $f \in E^r$, and the model is

$$z = Kf + \varepsilon.$$

Let Q be a given strictly positive definite r×r matrix with symmetric square root $Q^{1/2}$, and let the singular value decomposition of $KQ^{1/2} \stackrel{\text{def}}{=} \tilde{K}$ be

$$KQ^{1/2} = UDV',$$

where D is r×r with diagonal entries d_i and let $u_1,\ldots,u_r$ and $v_1,\ldots,v_r$ be the r columns of U and V respectively. The u_i are n-vectors and the v_i are r vectors. Not to worry, we are not actually going to compute U,D or V. The Q-generalized inverse solution $K_Q^+ z$ of the equation z = Kf is defined as that element f in E_r which minimizes $f'Q^{-1}f$ subject to $Kf = \hat{z}$, where $\hat{z}$ is the orthogonal projection of z onto the range of K. $K_Q^+ z$ is given by

$$K_Q^+ z = QK'(KQK')^+ z = Q^{1/2}\tilde{K}'(\tilde{K}\tilde{K}')^+ z$$

$$= \sum_{j:d_j \neq 0} \frac{(z,u_j)}{d_j} Q^{1/2} v_j$$

where "+" denotes the usual Moore-Penrose generalized inverse.

Now consider the generalized Landweber iteration

$$\begin{aligned} f^k &= f^{k-1} + \beta QK'(z - Kf^{k-1}), \quad k = 1,2,\ldots \\ &= (I - \beta QK'K)f^{k-1} + \beta QK'z \end{aligned} \tag{8.1}$$

with $f^0 = 0$.

It is necessary that β satisfies $\beta < 2/d_1^2$. Then

$$Q^{-1/2}f^k = (I - \beta Q^{1/2}K'KQ^{1/2})Q^{-1/2}f^{k-1} + \beta Q^{1/2}K'z.$$

Let

$$\tilde{f}^k = Q^{-1/2} f^k.$$
$$\tilde{K} = KQ^{1/2}.$$

Then

$$\tilde{f}^k = (I-\beta\tilde{K}'\tilde{K})\tilde{f}^{k-1} + \beta\tilde{K}'z \tag{8.2}$$

and for this (ordinary) Landweber iteration it is not hard to show, using the identity

$$[I+(I-B)+\ldots+(I-B)^{k-1}]B = I - (I-B)^k,$$

for symmetric matrices (see Miller (1974)) that

$$\tilde{f}^k = \sum_{j:d_j>0} (1-(1-\beta d_j^2)^{k-1})\frac{(z,u_j)}{d_j} v_j$$

hence

$$f^k = \sum_{j:d_j>0} (1-(1-\beta d_j^2)^{k-1})\frac{(z,u_j)}{d_j} Q^{1/2} v_j \tag{8.3}$$

To get f^k from $K_Q^+ z$, the component of $K_Q^+ z$ in the direction of $Q^{1/2}v_j$ is "damped" by the factor $(1-(1-\beta d_j^2)^{k-1})$, which decreases to 0 as d_j^2 decreases and clearly provides a useful form of regularization. For comparison, the minimizer of

$$\frac{1}{n}||z - Kf||^2 + \lambda f'Q^{-1}f$$

is

$$f_{n,\lambda} = \sum_{j:d_j^2>0} \frac{1}{1+n\lambda/d_j^2} \frac{(z,u_j)}{d_j} Q^{1/2} v_j$$

so that in the Landweber iteration the "damping factor" $(1-(1-\beta d_j^2)^{k-1})$ replaces the "damping factor" $1/(1+n\lambda/d_j^2)$ which occurs in regularization in the form in which we have been studying it earlier.

One can obtain the GCVF for f^k without solving for the d_j or u_j explicitly as follows: Since $KQ^{1/2}v_i = d_i u_i$, we have

$$Kf^k = \sum_{j:d_j>0} (1-(1-\beta d_j^2)^{k-1})(z,u_j)u_j. \tag{8.4}$$

This equation (8.4) defines the $n\times n$ matrix $A(k,\beta)$ which plays the role of $A(\lambda)$ in the GCVF. Here $A(k,\beta) = U\Lambda U'$, where Λ is the $r\times r$ diagonal matrix with jj^{th} entry $(1-(1-\beta d_j^2)^{k-1})$. Thus, the GCVF $V(k,\beta)$ is given by

$$V(k,\beta) = \frac{\frac{1}{n}\|z-Kf^k\|^2}{[\frac{1}{n}\mathrm{Tr}(I-\beta KQK')^{k-1}]^2}.$$

Assuming that $(I-\beta KQK')$ can be multipled by itself $k-1$ times, the GCVF can be computed for large problems of this type. One computes $V(1,\beta)$, $V(2,\beta)$,... until a minimum is found. The choice of Q is made, if possible, based on the belief that the true but unknown f has the property that $f'Q^{-1}f$ is relatively small. This is completely analogous to choosing an r.k.h.s. with r.k. $Q(s,t)$ with the belief that $\|f\|_Q^2$ is small, where $\|\cdot\|_Q$ is the norm induced by Q.

9. Acknowledgements

The author wishes to thank M.Z. Nashed for organizing the International Symposium on Ill Posed Problems, held at Newark, Delaware, October 2-6, 1979, where some of the ideas presented here had a chance to 'ferment". She also wishes to acknowledge the help of conversations with Gabor Herman, Bob Anderssen and Don Chambless, and the support of the Office of Naval Research.

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1. REPORT NUMBER: Technical Report No. 595 (9)	2. GOVT ACCESSION NO. / 3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle): Ill Posed Problems: Numerical and Statistical Methods for Mildly, Moderately and Severely Ill Posed Problems with Noisy Data (6)	5. TYPE OF REPORT & PERIOD COVERED: Scienfitic Interim 6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s): Grace Wahba (10)	8. CONTRACT OR GRANT NUMBER(s): (15) N00014-77-C-0675
9. PERFORMING ORGANIZATION NAME AND ADDRESS: Department of Statistics / University of Wisconsin, Madison / Madison, WI 53706	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS: Office of Naval Research / 800 North Quincy Street / Arlington, VA 22217 (12, 14)	12. REPORT DATE: (11) Feb[illegible]1980 13. NUMBER OF PAGES: 69
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)	15. SECURITY CLASS. (of this report): Unclassified 15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

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17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

(14) UWIS-DS-80-595

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Ill-posed problems, regularization, cross validation

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

(see reverse side)

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE
S/N 0102-LF-014-6601

Unclassified

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

400243

ABSTRACT

We discuss a number of topics related to the practical solution of ill posed problems given noisy data as it might arise in an experimental situation. The model is $z_i = \int_0^1 K(t_i,t)f(t)dt + \varepsilon_i$, $i = 1,2,\ldots,n$, where $z = (z_1,\ldots,z_n)'$ is the data vector, $\varepsilon = (\varepsilon_1,\ldots,\varepsilon_n)'$ is a vector of independent zero mean random variables with common unknown variance, K is known, and it is desired to estimate f given z. We first define the intrinsic rank of the problem where $\int_0^1 K(t_i,t)f(t)dt$ is known exactly. This definition is used to provide insight into the circumstances in which one may expect to estimate f well, moderately well, or poorly. The sensitivity of a regularized estimate of f to the noise is made explicit. After giving the intrinsic rank of the examples of first and second derivative, Abel's equation and Fujita's equation, it is argued that the first three are only mildly ill posed and f should be amenable to accurate estimation by the method of regularization. The method of Generalized Cross Validation (GCV) for choosing the regularization parameter is described and numerical results for the estimation of first and second derivative from noisy data are given. Two numerical algorithms for obtaining a regularized estimate with GCV are detailed. The second uses a B-spline basis to allow the handling of large data sets. The use of outside information in the estimation of f is discussed. Three types of outside information are of interest. 1) Several values of continuous linear functionals on f are known approximately, 2) this same information is given exactly and 3) f is known to be in a closed convex set, in particular f non-negative. The GCV estimate of the regularization parameter has to be modified in case 3) if the closed convex set is not a linear manifold. To do this we develop the notion of GCV for constrained problems. Next, we discuss the problem of checking the validity of the 'model' K, and provide a crude goodness-of-fit test. Finally we end by describing the (known) result that the number k of iterations in a Landweber iteration for solving large linear systems is a form of regularization parameter. We then show how GCV can feasibly be used to choose k in very large problems like those arising in computerized tomography.