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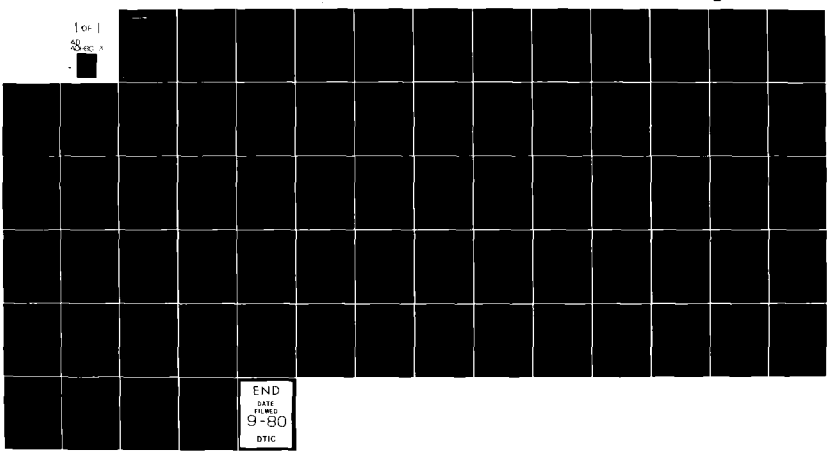

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NUMERICAL REGULARIZATION OF ILL-POSED PROBLEMS

C. W. Groetsch

Department of Mathematical Sciences

University of Cincinnati

Cincinnati, Ohio 45221

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

A number of results on general regularization methods for ill-posed linear problems and related mathematical ideas were developed during the course of the project. These results are documented in four papers, all of which have been accepted for publication. The investigator has taken the point of view of generalized inversion in studying numerical metnods for the regularization of ill-posed problems. Some ideas of A. Sard are extended to provide a general axiomatic framework for both splines (including interpolatory splines and generalized harmonic functions) and the Moore-Penrose generalized inverse.

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20. Abstract cont.

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Convergence theorems and error bounds for a very general class of regularization methods are developed in (3). The error bounds related the smoothness of the data to a modulus of convergence for the general regularization method (which includes as special cases both iterative and noniterative regularization methods). Work is in progress on inverse results which show that a certain rate of convergence for a regularization method implies a certain degree of smoothness for the data.

Paper (4) surveys, extendds and unifies the mathematical theory of parameter choice in linear regularization. Included are discussions of a priori parameter choice strategies, the Discrepancy Principle, the derivative and ratio-criteria, and a parameter choice criterion for approximating constrained pseudo-solutions.

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1. Generalized inverses and generalized splines; Numerical Functional Analysis and Optimization.
2. On the Kryanev-Lardy method for ill-posed problems; Mathematische Nachrichten.
3. On a class of regularization methods; Bolletino della Unione Matematica Italiana.
4. The parameter choice problem in linear regularization: a mathematical introduction, in "Ill-Posed Problems: Theory and Practice" (M.Z. Nashed, Ed.), Wiley, New York.

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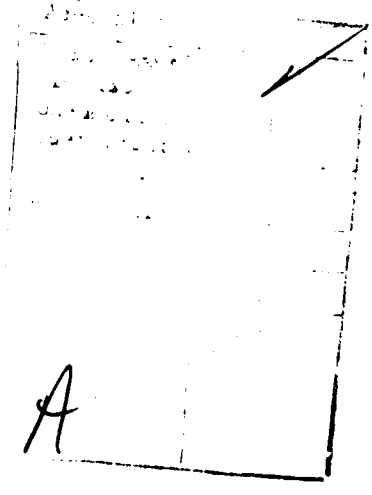
Complete copies of the papers follow as appendixes.



GENERALIZED INVERSES AND GENERALIZED SPLINES

C. W. Groetsch

Department of Mathematical Sciences
University of Cincinnati
Cincinnati, Ohio 45221

ABSTRACT

An abstract framework in Hilbert space is provided for generalized splines and generalized inverses of operators.

Since Atteia [1] introduced an abstract point of view in the theory of spline functions, a number of authors have studied abstract splines in Hilbert space and relationships between spline functions and generalized inverses (see [2], [3], [4], [6], [7]). In [7] Sard developed a very elegant theory of "splines" in Hilbert space. Our aim in this brief note is to enlarge somewhat the context introduced by Sard so as to provide a framework which encompasses the splines in the sense of Sard and also the concept of the generalized inverse of a linear operator in Hilbert space.

Suppose that X and W are linear spaces and that Y and Z are inner product spaces (the inner product and induced norm in each space will be denoted by $\langle \cdot,\cdot \rangle$ and $\|\cdot\|$, respectively). We also assume that there are two linear mappings

$$F : X \times W \to Z \quad \text{and} \quad U : X \times W \to Y$$

which satisfy

(1) $F(x,0) = 0$ and $U(x,0) = 0$ implies $x = 0$

and

(2) $F(0,w) = 0$ and $U(0,w) = 0$ implies $w = 0$.

These linear maps are the bivariate analogues of Sard's "observation" and "coobservation" operators (see [7]). By virtue of (1), the bilinear form

$$[x,y] = \langle F(x,0),F(y,0)\rangle + \langle U(x,0),U(y,0)\rangle$$

is an inner product on X and we will denote by $\overline{X}$ the Hilbert space which is the completion of X in the norm $|\cdot|$ induced by this inner product. Condition (2) guarantees that the bilinear form

$$(w,v) = \langle F(0,w),F(0,v)\rangle + \langle U(0,w),U(0,v)\rangle$$

is an inner product on W and we shall designate the completion of W with respect to this inner product by $\tilde{W}$. Note that the mappings F and U are continuous on $X \times W$ and we will persist in denoting the continuous extensions of these mappings to $\overline{X} \times \tilde{W}$ by F and U respectively. We assume that for each $b \in W$ the closed convex set $p(b)$ defined by

$$p(b) = \{x \in \overline{X} : F(x,b) = 0\}$$

is nonempty (note that $p(0)$ is a closed subspace of $\overline{X}$). One may view this requirement as an abstract "interpolation" condition. The symbol $\overline{W}$ will designate the subspace of $\tilde{W}$ which is maximal (relative to inclusion) with respect to the property that $p(b) \neq \emptyset$ for all $b \in \overline{W}$. Note that $W \subset \overline{W} \subset \tilde{W}$. As a final bit of notation, π will be the mapping which associates with each closed convex subset of $\overline{X}$ its unique element of minimal norm.

Definition. The mapping $b \to b^\dagger$ from $\overline{W}$ into $\overline{X}$ defined by $b^\dagger = \pi_0 p(b)$ will be called the generalized spline mapping associated with the structure (X,W,F,u).

Note that if we set $M = p(0)^\perp$, then one sees readily that $p(b) = b^\dagger + p(0)$ and $M \cap p(b) = \{b^\dagger\}$.

Proposition 1. If $b \in \overline{W}$, then $||u(x,0)||$ is minimal among all $x \in p(b)$ if and only if $x = b^\dagger$.

Proof. If $x \in p(b)$, then since $F(x,b) = 0$ and $F(b^\dagger,b) = 0$, we find that $x - b^\dagger \in p(0) = M^\perp$. Therefore

$$||u(x,0)||^2 + ||F(x,0)||^2 = |x|^2 = |x - b^\dagger|^2 + |b^\dagger|^2.$$

But since $F(x - b^\dagger,0) = 0$, it follows that $F(x,0) = F(b^\dagger,0)$ and hence

$$||u(x,0)||^2 = |x - b^\dagger|^2 + |b^\dagger|^2 - ||F(b^\dagger,0)||^2,$$

which establishes the assertion.

Proposition 2. The generalized spline mapping $b \to b^\dagger$ is a closed linear operator which is continuous if and only if $\overline{W}$ is complete.

Proof. The linearity follows easily from the fact that $p(b_1 + b_2) = \{x + y : x \in p(b_1),\ y \in p(b_2)\}$ and the representation $p(b) = b^\dagger + p(0)$. Suppose that $\{b_n\} \subset \overline{W}$ and $(b_n^\dagger, b_n) \to (x,b) \in \overline{X} \times \tilde{W}$. By the continuity of F, we then have

$$F(x,b) = \lim_n F(b_n^\dagger, b_n) = 0.$$

Therefore $x \in p(b)$ and hence $b \in \overline{W}$, by the maximality of $\overline{W}$. Also, since M is closed and $\{b_n^\dagger\} \subset M$, we have $x \in M \cap p(b) = \{b^\dagger\}$. Therefore the graph of the generalized spline mapping is closed, that is, the generalized spline mapping is a closed operator.

If $\overline{W}$ is complete then the generalized spline mapping is continuous by the Closed Graph Theorem. On the other hand, if the generalized spline mapping is continuous, then it has a continuous extension $b \to b^\#$ defined for all $b \in \tilde{W}$. Suppose $b \in \tilde{W}$ and choose a sequence $\{b_n\} \subset W$ with $b_n \to b$. Then, since F is continuous,

$$F(b^\#,b) = \lim_n F(b_n^\#,b_n) = \lim_n F(b_n^\dagger,b_n) = 0.$$

Therefore $p(b) \neq \emptyset$ and hence $b \in \overline{W}$. It follows that $\tilde{W} \subset \overline{W}$, that is, $\overline{W}$ is complete.

In the special case when $W = X$, $F(x,b) = Fx - Fb$ and $U(x,b) = Ux - Ub$, where F and U are linear operators, we recover Sard's theory of splines. Here $\overline{W} = \overline{X}$, $M = N(F)^\perp$ is the space of "splines" and $b^\dagger = P_M b$, the projection of b onto M, is the spline approximation to $b \in \overline{X}$. Proposition 1 is then just a statement of the "optimal interpolation" property of splines. For specific applications to interpolatory splines and generalized harmonic functions see [7].

As another example, suppose H_1 and H_2 are Hilbert spaces, D(T) is a dense subspace of H_1 and $T : D(T) \to H_2$ is a closed linear operator. Let Q be the orthogonal projection of H_2 into $\overline{R(T)}$. Let $X = D(T)$, $W = R(T) + R(T)^\perp$, $Z = H_2$ and $Y = H_1 \times H_2$. Define the linear operators $F : X \times W \to Z$ and $U : X \times W \to Y$ by $F(x,b) = Tx - Qb$ and $U(x,b) = (x,b)$. In this case $\overline{X} = D(T)$, $\overline{W} = W$, $p(b)$ is the set of least squares solutions of the equation $Tx = b$ and $b^\dagger = T^\dagger b$, where $T^\dagger$ is the Moore-Penrose inverse of T (see e.g. [5]).

Proposition 1 in this case expresses the well-known extremal property of the Moore-Penrose inverse and Proposition 2 is the (somewhat less) well-known characterization of continuous Moore-Penrose inverses.

ACKNOWLEDGMENT

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On the Kryanev-Lardy Method for Ill-Posed Problems[†]

C. W. Groetsch

1. Introduction.

Kryanev's method for solving the ill-posed operator equation

$$Au = f \quad , \tag{1}$$

where A is a linear operator on a real Hilbert space, consists of choosing a bounded, positive definite operator B and forming the sequence of iterates defined by

$$x_0 = 0 \quad , \quad Ax_n + Bx_n = Bx_{n-1} + f \quad . \tag{2}$$

Krayanev [3] established the convergence of the method under the assumption that A is a bounded positive semi-definite operator and equation (1) has a unique solution. The author [2] proved the convergence of a related method in the case when A is a densely defined closed linear operator, again under the assumption that for a given f equation (1) has a unique solution. Our aim in this note is to investigate the convergence of the method to a generalized solution of (1) when A is a closed unbounded operator and the existence of a unique solution is not assumed.

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2. Results.

Suppose that H_1 and H_2 are real Hilbert spaces (the inner product in each space will be designated by $\langle \cdot, \cdot \rangle$) and that $D(A)$ is a dense subspace of H_1. Let $A : D(A) \to H_2$ be a closed linear operator. We shall investigate an iterative method for approximating $A^\dagger f$, where $A^\dagger$ is the Moore-Penrose generalized inverse of A. We recall that $A^\dagger$ is the closed linear operator defined on the dense subspace

$$D(A^\dagger) = R(A) \oplus R(A)^\perp$$

of H_2 by $A^\dagger f = u$, where u is the solution of minimal norm of the equation

$$Ax = Qf \quad , \tag{3}$$

and Q is the orthogonal projection of H_2 onto $\overline{R(A)}$. We note that this definition of the generalized inverse is the same as that for a bounded operator (see e.g. [1]) and that for $f \in D(A^\dagger)$ the set of solutions of (3) is convex, nonempty and closed (since A is closed). Therefore the vector $A^\dagger f$ is uniquely defined.

We shall suppose that $B : H_1 \to H_1$ is a bounded, self-adjoint operator satisfying

$$\langle Bx, x \rangle \geq c^2 \, ||x||^2 \tag{4}$$

for all $x \in H_1$ and some $c \neq 0$. We may define an equivalent inner product

on H_1 by

$$[x,y] = \langle Bx,y\rangle \ ,$$

and we shall denote the Hilbert space which consists of H_1 with the new inner product $[\cdot,\cdot]$ by H_1. The norm in H_1 will be denoted $||\cdot||_B$, that is

$$||x||_B^2 = \langle Bx,x\rangle = [x,x] \ .$$

Since the norms $||\cdot||$ and $||\cdot||_B$ are equivalent, the subspace D(A) is also dense in H_1. The adjoint of A considered as an operator on H_1 will be designated by A'. That is,

$$A' : D(A') \to H_1$$

satisfies $\langle Ax,y\rangle = [x,A'y]$

for all $y \in D(A') = \{y \in H_2 : \langle Ax,y\rangle = [x,z]$, some $z \in H_2$ and all $x \in D(A)\}$. The adjoint of A considered as an operator on H_1 will be designated by the customary symbol, A^*. Note that these two adjoints are related in a simple way. Namely, $D(A') = D(A^*)$ and $A^* = BA'$. By [5, page 307] the operator

$$(I_1 + A'A)^{-1} : H_1 \to H_1 \ ,$$

where I_1 is the identity operator on H_1, is a bounded, self-adjoint operator on H_1 satisfying

$$(5) \qquad ||(I_1 + A'A)^{-1}||_B \leq 1 \quad .$$

Lemma 1. Given $f \in H_2$, there is a unique $u_1 \in D(A)$ such that

$$<Bu_1,v> + <Au_1,Av> = <f,Av>$$

for all $v \in D(A)$. Moreover, if $f \in D(A^\dagger)$, then $u_1 = u - Wu$, where $W = (I_1 + A'A)^{-1}$ and $u = A^\dagger f$.

Proof. Since A is closed, D(A) is a Hilbert space under the inner product $(\cdot,\cdot)$ defined by

$$(x,y) = [x,y] + <Ax,Ay> \quad .$$

The linear functional ϕ defined on D(A) by $\phi(v) = <f,Av>$ is clearly continuous with respect to the norm induced by the inner product $(\cdot,\cdot)$. Therefore, by the Riesz Theorem, there is a unique $u_1 \in D(A)$ with

$$<f,Av> = \phi(v) = (u_1,v)$$

for all $v \in D(A)$, which was to be shown.

If $f \in D(A^\dagger)$ and $u = A^\dagger f$, then $Au = Qf$, and since $<f,Av> = <Qf,Av>$ for all $v \in D(A)$ and $Wu \in D(A^*A)$, we have

$$\langle B(u - Wu), v\rangle + \langle A(u - Wu), Av\rangle$$

$$= \langle Bu, v\rangle - \langle BWu, v\rangle - \langle AWu, Av\rangle + \langle Au, Av\rangle$$

$$= \langle Bu, v\rangle - \langle (B + A^*A)Wu, v\rangle + \langle Qf, Av\rangle$$

$$= \langle Bu, v\rangle - \langle B(I_1 + A'A)Wu, v\rangle + \langle f, Av\rangle = \langle f, Av\rangle \quad .$$

But then, by the first part of the Lemma, $u_1 = u - Wu$, which was to be proved.

We will study the sequence of iterates defined by

$$(6) \qquad u_n = Wu_{n-1} + u_1 \quad , \quad n = 1,2,3,\ldots$$

where u_1 is given by Lemma 1. Note that this is equivalent to the requirement that

$$\langle Bu_n, v\rangle + \langle Au_n, Av\rangle = \langle Bu_{n-1}, v\rangle + \langle f, Av\rangle$$

for all $v \in D(A)$, which establishes the connection with Kryanev's method. This can be established exactly as in the proof of Lemma 1 by considering the linear functional

$$\phi(v) = \langle Bu_{n-1}, v\rangle + \langle f, Av\rangle$$

on the Hilbert space $D(A)$. In the case $B = I$ and $f \in D(A^\dagger)$, the method (6) reduces to that investigated by Lardy [4].

Lemma 2. If $f \in D(A^\dagger)$ and $u = A^\dagger f$, then $u - u_n = W^n u$.

Proof. By (6) and Lemma 1, we have

$$u - u_n = u - u_1 - Wu_{n-1} = u - (u - Wu) - Wu_{n-1}$$

$$= W(u - u_{n-1}) \quad .$$

Therefore, $u - u_n = W^n u$, $n = 1,2,3,\ldots$.

We may now provide an error bound for the method (6). For convenience we will henceforth denote the operator A^*A by $\tilde{A}$.

Theorem 1. Suppose $R(\tilde{A}) \subseteq R(A'A)$ and $Qf = A\tilde{A}z$ for some $z \in H_1$, then for some $y \in H_1$,

$$||u - u_n||_B^2 \leq \frac{1}{n-1}\left(1 - \frac{1}{n}\right)^n ||y||_B^2 \quad , \quad \text{for } n > 1 \quad .$$

Proof. Since $R(\tilde{A}) \subseteq R(A'A)$, we have $\tilde{A}z = A'Ay$, for some $y \in H_1$. Let $\{E_\lambda\}$ be the resolution of the identity in H_1 induced by the self-adjoint operator $A'A$. Since $Qf = A\tilde{A}z$ and $\tilde{A}z \in N(A)^\perp$, we have $\tilde{A}z = A^\dagger f$. Therefore by Lemma 2,

$$u - u_n = W^n A'Ay = \int_0^\infty \frac{\lambda}{(1+\lambda)^n}\, dE_\lambda y \quad .$$

It then follows that

$$\|u - u_n\|_B^2 = \int_0^\infty \frac{\lambda}{(1+\lambda)^n} d[E_\lambda y, y]$$

$$\leq \frac{1}{n-1}\left(1 - \frac{1}{n}\right)^n \int_0^\infty d[E_\lambda y, y]$$

$$= \frac{1}{n-1}\left(1 - \frac{1}{n}\right)^n \|y\|_B^2 \quad .$$

We note that if we make the weaker assumption that $f \in D(A^\dagger)$ (i.e. $Qf \in R(A)$), rather than the stronger assumption that $Qf \in R(A\tilde{A})$, then the method still converges. For in this case we have by Lemma 2,

$$\|u - u_n\|_B^2 = \int_0^\infty (1+\lambda)^{-n} d[E_\lambda u, u] \to 0 \quad \text{as} \quad n \to \infty \ .$$

However, if $f \notin D(A^\dagger)$, then the sequence $\{u_n\}$ diverges and in fact has no weakly convergent subsequence. For if the subsequence $\{u_{n_k}\}$ converges weakly to y, then since W is bounded and therefore weakly continuous, we have by (6)

$$y - Wy = u_1 \quad . \tag{7}$$

Since $u_1 \in D(A)$ and $Wy \in D(\tilde{A}) \subset D(A)$, we find that $y \in D(A)$. Also, by Lemma 1 and (7)

$$\langle f, Av\rangle = \langle By - BWy, v\rangle + \langle Ay - AWy, Av\rangle$$

$$= \langle By, v\rangle - \langle (B + \tilde{A})Wy, v\rangle + \langle Ay, Av\rangle$$

$$= \langle Ay, Av\rangle \quad , \quad \text{for all } v \in D(A) \quad .$$

Therefore, $f - Ay \in R(A)^{\perp}$, that is, $f \in D(A^{\dagger})$. We summarize these results in the following:

Theorem 2. If $f \in D(A^{\dagger})$, then $u_n \to A^{\dagger}f$. However, if $f \notin D(A^{\dagger})$, then $\{u_n\}$ has no weakly convergent subsequence.

Since bounded sets in Hilbert space are weakly compact, we obtain immediately the following:

Corollary. If $f \notin D(A^{\dagger})$, then $||u_n|| \to \infty$.

Finally, we investigate the method under the assumption that the exact data f is unavailable, but an approximation $\tilde{f}$ satisfying $||f - \tilde{f}|| \leq \delta$ is on hand. The first approximation $\tilde{u}_1$ (corresponding to the corrupted data $\tilde{f}$) then satisfies

$$(\tilde{u}_1, v) = \langle B\tilde{u}_1, v\rangle + \langle A\tilde{u}_1, Av\rangle = \langle \tilde{f}, Av\rangle$$

for all $v \in D(A)$. By Lemma 1 we then have

$$(u_1 - \tilde{u}_1, v) = \langle f - \tilde{f}, Av\rangle$$

for all $v \in D(A)$. Setting $v = u_1 - \tilde{u}_1$, this gives

$$(8) \qquad (u_1 - \tilde{u}_1,\ u_1 - \tilde{u}_1) = \langle f - \tilde{f},\ A(u_1 - \tilde{u}_1)\rangle \quad .$$

If we designate the norm on $D(A)$ induced by the inner product $(\cdot,\cdot)$ by $||\cdot||_1$, then we have

$$||Ax||^2 \le \langle Bx,x\rangle + \langle Ax,Ax\rangle = ||x||_1^2$$

for all $x \in D(A)$. Therefore by (8), it follows that

$$||u_1 - \tilde{u}_1||_1^2 \le ||f - \tilde{f}||\ ||A(u_1 - \tilde{u}_1)||^2 \le \delta||u_1 - \tilde{u}_1||_1$$

and hence

$$||u_1 - \tilde{u}_1||_B \le ||u_1 - \tilde{u}_1||_1 \le \delta.$$

Later approximations using the data $\tilde{f}$ satisfy by (6)

$$\tilde{u}_n = W\tilde{u}_{n-1} + \tilde{u}_1,$$

and therefore

$$u_n - \tilde{u}_n = \sum_{k=0}^{n-1} W^k(u_1 - \tilde{u}_1) \quad , \quad n = 1,2,3,\ldots \ .$$

But $||W||_B \leq 1$, by (5), and therefore

$$||u_n - \tilde{u}_n||_B \leq n||u_1 - \tilde{u}_1||_B \leq n\delta.$$

It then follows that

$$||\tilde{u}_n - u||_B \leq ||\tilde{u}_n - u_n||_B + ||u_n - u||_B \leq n\delta + ||u_n - u||_B.$$

But $||u_n - u||_B \to 0$ as $n \to \infty$ if $f \in D(A^\dagger)$. Therefore, given $\epsilon > 0$ there is a $\delta(\epsilon)$ and n_ϵ such that

$$||\tilde{u}_{n_\epsilon} - u||_B < \epsilon \quad \text{for} \quad 0 < \delta \leq \delta(\epsilon),$$

that is, the method is a regularizing algorithm in the sense of Tikhonov (see [6]) if $f \in D(A^\dagger)$.

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Department of Mathematical Sciences
University of Cincinnati
Cincinnati, Ohio 45221
U.S.A.

On a Class of Regularization Methods[†]

C. W. Groetsch (Cincinnati)

Zusammenfassung

Wir studieren eine allgemeine Klasse von Regularisierungsmethoden für eine inkorrekt gestellte lineare Operatorgleichung im Hilbertsraum.

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On a Class of Regularization Methods[†]

C. W. Groetsch

In this note we will investigate a general class of regularization methods for the ill-posed operator equation

$$Tx = b \tag{1}$$

where T is a bounded linear operator from the Hilbert space H_1 into the Hilbert space H_2. The Moore-Penrose generalized inverse of T will be denoted by $T^\dagger$, that is $T^\dagger : \mathcal{D}(T^\dagger) \to H_1$ is the linear operator which associates with each vector $b \in \mathcal{D}(T^\dagger) := R(T) \oplus R(T)^\perp$ the unique least squares solution of minimal norm of equation (1) (see e.g. [3]). By a least squares solution of (1) we mean any solution of the equation

$$T^*Tx = T^*b, \tag{2}$$

where T^* is the adjoint of T. We will denote the operator T^*T by $\tilde{T}$ and the operator TT^* by $\hat{T}$. Note that $\tilde{T}$ and $\hat{T}$ are self-adjoint linear operators whose spectra lie in the interval $[0, ||T||^2]$. If $0 \notin \sigma(\tilde{T})$ (the spectrum of $\tilde{T}$), then by (2) we have $T^\dagger = \tilde{T}^{-1}T^*$. In general, however, $0 \in \sigma(\tilde{T})$, but this last equation nevertheless leads us to seek approximations to $T^\dagger$ by operators of the form $U(\tilde{T})T^*$ where U is a continuous function on $[0, ||T||^2]$ which approximates the function $f(t) = t^{-1}$ in some sense. Specifically, we will consider a family (net) of real valued functions $\{U_\beta(t) : \beta \in S\}$, indexed by a subset S of the positive real numbers with $\infty \in \overline{S}$, where each U_β is continuous on $[0, ||T||^2]$ and such that

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(3) $|tU_\beta(t)| \leq M$ for all t and β

and

(4) $U_\beta(t) \to t^{-1}$ as $\beta \to \infty$ for each $t \neq 0$.

Such a class of regularization methods for equation (1) was studied previously by Bakushinskii [1] under the assumption that $b \in R(T)$. (The author was unaware of Bakushinskii's studies when this research was performed.)

The following is proved in [3].

Proposition 1. Suppose $b \in \mathcal{D}(T^\dagger)$ and let $x_\beta = U_\beta(\tilde{T})T^*b$. Then $x_\beta \to T^\dagger b$ as $\beta \to \infty$.

To this we now add,

Proposition 2. If $b \notin \mathcal{D}(T^\dagger)$, then $\{x_\beta\}$ has no weakly convergent subnet and hence $||x_\beta|| \to \infty$ as $\beta \to \infty$.

Proof. Suppose $\{x_{\beta'}\}$ is a subnet of $\{x_\beta\}$ which converges weakly to $z \in H_1$, denoted $x_{\beta'} \overset{w}{\to} z$. By the weak continuity of bounded linear operators we then have $Tx_{\beta'} \overset{w}{\to} Tz$. Now, if we denote the projection of H_2 onto $\overline{R(T)}$ by P, then

$$\begin{aligned} Pb - Tx_\beta &= Pb - TU_\beta(\tilde{T})T^*b \\ &= Pb - \hat{T}U_\beta(\hat{T})Pb. \end{aligned}$$

However, by (3) and (4), the operator $\hat{T}U_\beta(\hat{T})$ converges pointwise to the projection of H_2 onto $N(\hat{T})^\perp = N(T^*)^\perp = \overline{R(T)}$. Therefore $Pb - Tx_{\beta'} \to 0$. It then follows that $Pb = Tz$, a contradiction. #

In the proof above we have used the fact that $U_\beta(\tilde{T})T^* = T^*U_\beta(\hat{T})$. This is easy to see if U_β is a polynomial. In the general case the identity follows from the Weierstrass approximation theorem.

Several authors have established rates of convergence for various approximations to $T^{\dagger}b$ under the stronger assumption that $Pb \in R(\hat{T})$ (see [9], [5], [6]). We see from Proposition 2 that the very least we must require to get convergence at all is that $b \in \mathcal{D}(T^{\dagger})$, i.e., $Pb \in R(T)$. In order to strengthen this condition only slightly and thereby obtain a rate of convergence we note that

$$R(T) = R(TP_{N(T)^{\perp}})$$

and, in the pointwise sense,

$$P_{N(T)^{\perp}} = \lim_{\nu \to 0^+} \tilde{T}^{\nu}.$$

It therefore seems reasonable to replace the hypothesis $b \in \mathcal{D}(T^{\dagger})$, i.e., $Pb \in R(T)$, by the hypothesis $Pb \in R(T\tilde{T}^{\nu})$ for some $\nu > 0$. In order to gauge the rate of convergence we will replace (3) by the stronger condition

$$(5) \qquad t^{\nu}|1 - tU_{\beta}(t)| \leq \omega(\beta,\nu) \qquad \text{for } \nu > 0$$

where $\omega(\beta,\nu) \to 0$ as $\beta \to \infty$ for each $\nu > 0$ (the case $\nu = 1$ was considered in [4]). The proof of the following lemma, being routine, is omitted.

Lemma 1. If $\nu > 0$, then $R(\tilde{T}^{\nu}) \subset N(T)^{\perp}$.

We now state a rate of convergence result. The vector $T^{\dagger}b$ will be denoted by x and the error $x - x_{\beta}$ by e_{β}.

Proposition 3. If $Pb = T\tilde{T}^{\nu}w$, where $\nu > 0$, then $||e_{\beta}|| \leq \omega(\beta,\nu)||w||$.

Proof. Since $Tx = Pb = T\tilde{T}^{\nu}w$ and since $x - \tilde{T}^{\nu}w \in N(T)^{\perp}$, we see that $x = \tilde{T}^{\nu}w$. Now,

$$\begin{aligned} x_{\beta} &= U_{\beta}(\tilde{T})T^{*}b = U_{\beta}(\tilde{T})T^{*}Pb \\ &= U_{\beta}(\tilde{T})\tilde{T}x = U_{\beta}(\tilde{T})\tilde{T}^{\nu+1}w. \end{aligned}$$

Therefore $e_\beta = x - x_\beta = \tilde{T}^\nu(I - U_\beta(\tilde{T})\tilde{T})w$. By the Spectral Mapping Theorem and Radius Formula, we then have

$$||e_\beta|| \leq \omega(\beta,\nu)||w||. \quad \#$$

In our next result we become more cavalier in our assumptions on the data.

Lemma 2. If $Pb = \hat{T}^\nu w$ where $\nu \geq 1$, then $||e_\beta||^2 \leq \omega(\beta,\nu-1)||Te_\beta||\,||w||$.

Proof. As in the previous proof we find that $x = T^*\hat{T}^{\nu-1}w$. Also,

$$x_\beta = U_\beta(\tilde{T})T^*Pb = U_\beta(\tilde{T})T^*\hat{T}^\nu w$$
$$= T^*U_\beta(\hat{T})\hat{T}^\nu w.$$

Therefore $e_\beta = x - x_\beta = T^*(I - U_\beta(\hat{T})\hat{T})\hat{T}^{\nu-1}w$, and

$$||e_\beta||^2 = (e_\beta, T^*(I - U_\beta(\hat{T})\hat{T})\hat{T}^{\nu-1}w$$
$$= (Te_\beta, (I - U_\beta(\hat{T})\hat{T})\hat{T}^{\nu-1}w) \leq \omega(\beta,\nu-1)||w||\,||Te_\beta||. \quad \#$$

Proposition 4. If $Pb = \hat{T}^\nu w$ where $\nu \geq 1$, then $||e_\beta||^2 \leq \omega(\beta,\nu)\omega(\beta,\nu-1)||w||$.

Proof. In Lemma 2 we saw that

$$e_\beta = T^*(I - U_\beta(\hat{T})\hat{T})\hat{T}^{\nu-1}w,$$

therefore

$$\tilde{T}e_\beta = T^*T^\nu(I - U_\beta(\hat{T})\hat{T})w.$$

We then have

$$||Te_\beta||^2 = (\tilde{T}e_\beta, e_\beta) = (T^\nu(I - U_\beta(\hat{T})\hat{T}w, Te_\beta)$$
$$\leq \omega(\beta,\nu)||Te_\beta||, \quad \text{i.e.,} \quad ||Te_\beta|| \leq \omega(\beta,\nu).$$

Substituting into the result of Lemma 2 completes the proof. #

In the next section we will give a number of examples of specific computational techniques to which the above results apply.

We have avoided for long enough the problem of polluted data. We now take up this question. Suppose that the data b is the result of measurements so that instead of b we have in our possession a corrupted version b^ε satisfying $||b - b^\varepsilon|| \leq \varepsilon$. We operate on the vector b^ε to obtain the approximations x_β^ε given by

$$x_\beta^\varepsilon = U_\beta(\tilde{T})T^* b^\varepsilon.$$

Let $\phi(\beta) = \sup\{|tU_\beta(t)| : t \in [0,||T||^2]\}$, and recall that $\phi(\beta)$ is bounded (by (3)).

Lemma 3. $||Tx_\beta - Tx_\beta^\varepsilon|| \leq \varepsilon\,\phi(\beta)$.

Proof. $\tilde{T}(x_\beta - x_\beta^\varepsilon) = \tilde{T}U_\beta(\tilde{T})T^*(b - b^\varepsilon)$, therefore

$$\begin{aligned} ||Tx_\beta - Tx_\beta^\varepsilon||^2 &= (\tilde{T}(x_\beta - x_\beta^\varepsilon), x_\beta - x_\beta^\varepsilon) \\ &= (\tilde{T}U_\beta(\tilde{T})T^*(b - b^\varepsilon), x_\beta - x_\beta^\varepsilon) \\ &= (\hat{T}U_\beta(\hat{T})(b - b^\varepsilon), T(x_\beta - x_\beta^\varepsilon)) \\ &\leq \phi(\beta)||b - b^\varepsilon||\;||T(x_\beta - x_\beta^\varepsilon)|| \\ &\leq \varepsilon\phi(\beta)||Tx_\beta - Tx_\beta^\varepsilon||. \quad \# \end{aligned}$$

Suppose now that $g(\beta) = \sup\{|U_\beta(t)| : t \in [0,||T||^2]\}$. We note that

(6) $$g(\beta) \to \infty \quad \text{as} \quad \beta \to \infty \ .$$

Indeed, if this were not the case, then there would be a constant L such that $|U_\beta(t)| < L$ for all t and β. But then $|tU_\beta(t)| \leq Lt \to 0$ as $t \to 0$, contradicting (4).

Lemma 4. $||x_\beta - x_\beta^\varepsilon|| \leq \varepsilon\sqrt{g(\beta)\phi(\beta)}$.

Proof. Since $x_\beta - x_\beta^\varepsilon = T^* U_\beta(\hat{T})(b - b^\varepsilon)$, we have, by use of Lemma 3,

$$||x_\beta - x_\beta^\varepsilon||^2 = (x_\beta - x_\beta^\varepsilon, T^* U_\beta(\hat{T})(b - b^\varepsilon))$$
$$= (T(x_\beta - x_\beta^\varepsilon), U_\beta(\hat{T})(b - b^\varepsilon))$$
$$\leq \varepsilon^2 \phi(\beta) g(\beta). \quad \#$$

Suppose how that $Pb = \hat{T}w$ (we could also use the other hypotheses considered above, but we choose to consider this simple case to illustrate the ideas). By the triangle inequality we have

$$||x - x_\beta^\varepsilon|| \leq ||x - x_\beta|| + ||x_\beta - x_\beta^\varepsilon||.$$

Lemma 4 and Proposition 4, then give

Proposition 5. If $Pb = \hat{T}w$, then

$$||x - x_\beta^\varepsilon|| \leq (||w|| \omega(\beta,1)\omega(\beta,0))^{\frac{1}{2}} + \varepsilon(g(\beta)\phi(\beta))^{\frac{1}{2}}.$$

The first term on the right hand side of this inequality goes to zero as $\beta \to \infty$. However, by (6) and (4), the second term becomes infinitely large as $\beta \to \infty$. This illustrates the classis dilemma in the numerical treatment of ill-posed problems. Even if computations are performed exactly, small errors in the data may eventually grow and overpower the approximations.

EXAMPLES

In this section we will consider some specific choices for the functions $\{U_\beta(t)\}$ and we will find functions $\omega(\beta,\nu)$ which determine rates of convergence. The index set S in all examples below will be either the set of nonnegative reals or nonnegative integers. In the discrete case, the parameter β will be denoted by n.

As a first example we consider Showalter's integral formula [8]:

$$T^\dagger b = \int_0^\infty \exp(-u\tilde{T})T^* b\, du.$$

The functions U_β for this example have the form

$$U_\beta(t) = \int_0^\beta \exp(-ut)du$$

and may be motivated in terms of Borel summability [3]. It is not difficult to see that a function $\omega(\beta,\nu)$ satisfying (5) is given by

$$\omega(\beta,\nu) = \beta^{-\nu} \quad (\nu > 0).$$

The choice $U_\beta(t) = (t + \beta^{-1})^{-1}$ $(\beta > 0)$ leads to Tychonov's regularization of order zero (see [1] and [10]). Here one can readily verify that

$$\omega(\beta,\nu) = \beta^{-\nu} \quad \text{for } 0 < \nu \leq 1.$$

In order to obtain approximations with this rate for $\nu > 1$ we may use extrapolated regularization [5]. That is, for a given $\beta > 0$ we set

$$U_\beta^{(0)}(t) = (t + \beta^{-1})^{-1}$$

and define Richardson extrapolants by

$$U_\beta^{(j)}(t) = (2^j U_{2\beta}^{(j-1)}(t) - U_\beta^{(j-1)}(t))/(2^j - 1), \quad j = 1,2,\ldots .$$

It is not difficult to show (see [5, Lemma 2.1]) that for $k = 0,1,2,\ldots$

$$t^{k+1}|1 - tU_\beta^{(k)}(t)| = \prod_{i=0}^{k} \left(\frac{t}{2^i\beta t + 1}\right)$$

$$\leq \beta^{-k-1}$$

Therefore, for the kth extrapolant we may apply Theorem 4 with $\omega(\beta,k) = \beta^{-k-1}$, $k = 1,2,\ldots$, to obtain the rate $\beta^{-k+\frac{1}{2}}$ (see [5, Theorem 3.2]).

We now consider some iterative regularization methods. Below, α will be a parameter satisfying $0 < \alpha < 2||T||^{-2}$.

If the functions $U_n(t)$, $n = 0,1,2,\ldots$ are defined

$$U_n(t) = \alpha \sum_{k=0}^{n} (1 - \alpha t)^k$$

then (3) and (4) are satisfied and one can show that

$$n^{\nu}t^{\nu}|1 - tU_n(t)| = n^{\nu}t^{\nu}|1 - \alpha t|^{n+1}$$

is uniformly bounded. From this we find that the rate of convergence of the iterative process

$$x_0 = \alpha T^* b, \quad x_{n+1} = (I - \alpha \tilde{T})x_n + \alpha T^* b$$

is determined by the function $\omega(n,\nu) = n^{-\nu}$.

Newton's method for approximating t^{-1} leads to the sequence of functions defined by

$$U_0(t) = \alpha, \; U_{n+1}(t) = U_n(t)(2 - tU_n(t)).$$

For this sequence of functions it is not difficult to see that

$$t^{\nu}|1 - tU_n(t)| = O(2^{-\nu n}) \quad \text{for} \quad \nu > 0.$$

Therefore the rate of convergence of the corresponding iterative method is determined by the function $\omega(n,\nu) = 2^{-\nu n}$.

Showalter and Ben-Israel [9] have extrapolated on the previous method to obtain methods with a higher rate of convergence. For a positive integer $p \geq 2$ they define the hyperpower methods in terms of the sequence

$$U_0(t) = \alpha, \; U_{n+1}(t) = U_n(t) \sum_{k=0}^{p-1} (1 - tU_n(t))^k.$$

For these methods the results above may be used to obtain the convergence rate $O(p^{-\nu n})$.

In [2] the following Krayanev-type method [7] is studied

$$x_0 = 0,\ \tilde{T}x_n + \beta^{-1}x_n = \beta^{-1}x_{n-1} + T^*b \qquad (\beta > 0).$$

One can verify, as in the first iterative example above, that the function $\omega(n,\nu) = (\beta n)^{-\nu}$ determines a rate of convergence.

The iterative method

$$x_0 = T^*b,\ x_{n+1} = x_n + (T^*b - \tilde{T}x_n)/(n+2),$$

was investigated in [6]. Following the analysis given in [6] one can show that the rate of convergence of this method is governed by the function $\omega(n,\nu) = (\log n)^{-\nu}$.

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Department of Mathematical Sciences
University of Cincinnati
Cincinnati, Ohio 45221 U.S.A.

THE PARAMETER CHOICE PROBLEM IN LINEAR REGULARIZATION: A MATHEMATICAL INTRODUCTION

C. W. Groetsch

1. INTRODUCTION

The concept of well-posedness for an equation of the form

$$Tx = b \tag{1.1}$$

was formulated at the turn of the century by Hadamard. The equation (or problem) (1.1) is said to be well-posed in the sense of Hadamard if for each b the equation has a unique solution and this solution depends continuously on b. If T is a transformation from a topological space X into a topological space Y, then the idea of well-posedness may be dissected by noting that the following three conditions on the triple (T,X,Y) are required:

(i) for each $b \in Y$, equation (1.1) has a solution,

(ii) the solution x is unique,

and (iii) the mapping $b \to x$ is continuous.

In this formulation it is evident that the well-posedness of (1.1) depends not only on T but is also intimately connected with the spaces X and Y and the topologies that they carry. Obviously, if the space Y is too broad, or if X is too narrow, then (i) cannot be satisfied. While if X is too large then (ii) will not hold. Moreover, if the topology of Y is too weak or that of X too strong, then (iii) will be violated.

In this exposition we shall restrict our attention to the case in which X and Y are Hilbert spaces and T is a bounded linear transformation from X to Y. With this context in mind, let us assume for the moment that for a given $b \in Y$ equation (1.1) has a solution. Condition (ii) will then hold if and only if $N(T) = \{0\}$ ($N(T) := \{x \in X: Tx = 0\}$ is the nullspace of T). If, however, $N(T) \neq \{0\}$, then (1.1) has infinitely many solutions, namely all vectors of the form $x + y$ where x is a particular solution and $y \in N(T)$. This family of solutions is clearly a closed convex set and therefore contains a unique member of smallest norm. An elementary geometrical argument characterizes this minimal norm solution as the unique solution which is normal (i.e. orthogonal) to $N(T)$. We will therefore call the minimal norm solution of (1.1) the normal solution. Since the normal solution is unique we see that (ii) is satisfied if we replace "solution" by "normal solution".

The normal solution exists of course only if $b \in R(T)$

$(R(T):=\{Tx:x\in X\}$ is the range of T). If $b \notin R(T)$ one might reasonably broaden one's notion of solution by seeking a vector in X which minimizes the functional

$$f(u) = ||Tu-b|| \quad .$$

It is a simple matter to show that the minima of f are precisely the solutions of the equation

$$Tx = Pb \tag{1.2}$$

where, here and henceforth, P denotes the orthogonal projection of the Hilbert space Y onto $\overline{R(T)}$, the closure of the range of T. Any solution of equation (1.2) will be called a pseudo-solution of (1.1). Equation (1.2) has a solution if and only if $Pb \in R(T)$ which is immediately seen to be equivalent to $b \in R(T) + R(T)^{\perp}$. Assuming that (1.2) is solvable, i.e. that $b \in R(T) + R(T)^{\perp}$, we will call the normal solution of (1.2) the pseudo-normal solution of equation (1.1). The operator which associates with each $b \in R(T) + R(T)^{\perp}$ the pseudo-normal solution of (1.1) is called the (Moore-Penrose) generalized inverse of the operator T. The generalized inverse of T, which is denoted by $T^{\dagger}$, has domain $\mathcal{D}(T^{\dagger}):= R(T) + R(T)^{\perp}$, which is a dense subspace of Y, and is a closed linear operator (see e.g. [20]). We therefore see that the triple $(T,N(T)^{\perp},\mathcal{D}(T^{\dagger}))$ satisfies (i) and (ii) if we are willing to extend our notion of "solution" to "pseudo-normal

solution". Moreover, the "solution operator" in this context is the generalized inverse $T^{\dagger}$. For further information on generalized inverses the reader may consult [6], [36], [50] and [20].

The scheme of things developed above does not however satisfy criterion (iii) (if it did there would be no linear ill-posed problems and this paper would not exist!). Indeed it is not difficult to show that the operator $T^{\dagger}$ is continuous if and only if $R(T)$ is closed (see e.g. [20]) and in the important example of Fredholm integral equations of the first kind the range is closed if and only if the kernel is degenerate, i.e. only quite rarely. We are therefore led to consider stable approximations to the pseudo-normal solution. A natural way to do this is to find bounded linear operators which approximate $T^{\dagger}$ in the pointwise sense. One approach to this problem is to view pseudo-solutions as solutions of the so-called normal equation

$$T^*Tx = T^*b \,, \tag{1.3}$$

where T^* is the adjoint of T. It is easy to show that equations (1.2) and (1.3) have the same solution sets (see e.g. [20]). If we denote, as we shall in the sequel, the self-adjoint operator T^*T by $\tilde{T}$, then we see that the set of all pseudo-solutions is $\tilde{T}^{-1} T^*b$. One might therefore reasonably attempt to form stable approximations to a pseudo-solution by

using vectors of the form $U_\alpha(\tilde{T})T^*b$, where $\{U_\alpha(t)\}_{\alpha>0}$ is a family of continuous real-valued functions on the spectrum of $\tilde{T}$ (which is contained in $[0,||T||^2]$) which approximates in some sense the function $t \to t^{-1}$. In [20], it is shown that if $|tU_\alpha(t)|$ is uniformly bounded and $U_\alpha(t) \to t^{-1}$ as $\alpha \to 0$ for each $t > 0$, then

$$x_\alpha := U_\alpha(\tilde{T})T^*b \to T^\dagger b$$

as $\alpha \to 0$ for each $b \in \mathcal{D}(T^\dagger)$. We shall call such a family of operators $\{U_\alpha(\tilde{T})T^*\}$ a regularizor of equation (1.1). This method of constructing regularizors via spectral theory was previously investigated in a somewhat different context by Bakushinskii [5]. We remark that the condition $b \in \mathcal{D}(T^\dagger)$ is also a necessary condition for the convergence of the regularizing algorithm. In fact, if $b \notin \mathcal{D}(T^\dagger)$ then it can be shown that $\{U_\alpha(\tilde{T})T^*b\}$ has no weakly convergent subnet [21].

From the practical viewpoint the crux of the difficulty with ill-posed problems is the fact that the right hand side is typically the result of measurements and is therefore only approximately determined. Since the solution operator is in general discontinuous, it then happens that small errors in the right hand side can lead to large variations in the computed solution. Specifically, if δ is some approximation to $b \in \mathcal{D}(T^\dagger)$ and the approximations $\hat{x}_\alpha$ are defined by

$$\hat{x}_\alpha := U_\alpha(\tilde{T})T^*\hat{b} \ ,$$

then one can establish the bound

$$||\hat{x}_\alpha - T^\dagger b|| \leq ||x_\alpha - T^\dagger b|| + ||b-\hat{b}|| \ (Mg(\alpha))^{1/2} \qquad (1.4)$$

where $|tU_\alpha(t)| \leq M$ and $g(\alpha) = \sup_t |U_\alpha(t)|$ (see [21]).

As has already been noted, the first term on the right hand side of this inequality tends to zero as $\alpha \to 0$, however, the hypotheses on the functions $\{U_\alpha(t)\}$ imply that $g(\alpha) \to \infty$ as $\alpha \to 0$. Therefore, this bound illustrates the typical dilemma in the numerical analysis of ill-posed problems: the error consists of two components, one of which is independent of the measured data and tends to zero while the other increases without bound for a fixed level of error in the input data. Too small of a choice of α, for a fixed level of error in the data, will consequently cause the quality of the computed approximations to be debased under the influence of this error. The effective numerical treatment of such problems therefore requires criteria which relate the regularization parameter to the error level in the input data in such a way that as the error tends to zero the regularized approximations $\hat{x}_\alpha$ tend to the pseudo-normal solution. The choice of a proper parameter is therefore in the words of Baker [3], "a practical detail of great relevance".

Thus the first step in the numerical solution of (1.1)

involves two essential choices: the selection of a regularizor and the choice of a criterion for selecting the regularization parameter. The regularizor which has been studied most extensively is the so-called Tikhonov [61] regularizor given by

$$U_\alpha(t) = (t+\alpha)^{-1}$$

(see also [53] and [66]). Our aim in the sequel is to give a theoretical presentation of various parameter choice strategies.

II. A Priori Parameter Choices

We shall suppose that $b \in \mathcal{D}(T^\dagger)$ and b^δ is some measured approximation to b satisfying $||b-b^\delta|| \leq \delta$ (this will be relaxed below). The actual approximations with which we are forced to work are given by

$$x_\alpha^\delta := U_\alpha(\tilde{T})T^*b^\delta$$

while the "idealized" approximations are

$$x_\alpha := U_\alpha(\tilde{T})T^*b \ .$$

The earliest parameter choice criteria involved some a priori choice of α depending on the error level, say $\alpha = \alpha(\delta)$, such that

$$||x_{\alpha(\delta)}^\delta - T^\dagger b|| \to 0 \quad \text{as} \quad \delta \to 0 \ .$$

Of course, the optimal choice would be some value $\alpha = \alpha_0$ satisfying

$$||x_{\alpha_0}^{\delta} - T^{\dagger}b|| = \inf_{\alpha>0} ||x_{\alpha}^{\delta} - T^{\dagger}b|| \quad ,$$

but such a value of the parameter is for practical purposes impossible to find. Alternatively, we might reconsider the bound (1.4) to obtain

$$||x_{\alpha}^{\delta} - T^{\dagger}b|| \leq ||x_{\alpha} - T^{\dagger}b|| + \delta(Mg(\alpha))^{1/2} \tag{2.1}$$

and seek a quasi-optimal value of α, that is a value which minimizes the right hand side. The difficulty here is that even an asymptotic bound for the quantity $||x_{\alpha} - T^{\dagger}b||$ usually requires information on the unknown vector b which is generally unavailable (see [21], [22]). Köckler [33] has shown however that in the case of Tikhonov regularization for matrices it may be possible to find an a posteriori estimate of the quasi-optimal parameter.

Leaving aside questions of optimality, we see from (2.1) that the method converges if we simply choose a value $\alpha(\delta)$ of α such that $\alpha(\delta) \to 0$ and $\delta(Mg(\alpha(\delta)))^{1/2} \to 0$ as $\delta \to 0$. In the special case of Tikhonov regularization, i.e. $U_{\alpha}(t) = (t+\alpha)^{-1}$, we have $M = 1$ and $g(\alpha) = \alpha^{-1}$ and therefore a sufficient condition for convergence is $\alpha \to 0$ and $\delta/\sqrt{\alpha} \to 0$ as $\delta \to 0$. Phrasing this slightly differently, if we choose positive functions $\beta_1(\delta)$ and $\beta_2(\delta)$ which converge to zero as $\delta \to 0$ and take α so that $\beta_2(\delta) \geq \alpha$ and $\delta/\sqrt{\alpha} \leq \sqrt{\beta_1(\delta)}$, that is,

$$\delta^2/\beta_1(\delta) \leq \alpha \leq \beta_2(\delta) , \tag{2.2}$$

then convergence is assured. The formulation (2.2) appears in Tikhonov and Arsenin [64].

For the remainder of this paper we will be concerned exclusively with the Tikhonov regularizor. During the past decade and a half the analytical theory of Tikhonov regularization has been developed to a very high level. The success of this effort is due largely to the fact that the Tikhonov regularizor, unlike the general class of regularizors considered in the introduction, possesses a very simple and natural variational property. Recall that our goal is to approximate the pseudo-normal solution, that is, the vector x satisfying

$$Tx = Pb$$

for which $||x||$ is minimal. In other words, we wish to minimize $||x||^2$ subject to the constraint $||Tx-Pb||^2 = 0$. Since $I-P$ is the orthogonal projector of Y onto $R(T)^{\perp}$ we have

$$||Tx-b||^2 = ||Tx-Pb||^2 + ||(I-P)b||^2$$

and hence we wish to minimize $||x||^2$ subject to $||Tx-b||^2 = ||(I-P)b||^2$. Classical Lagrange multiplier theory leads us to consider the functional

$$\lambda||Tx-b||^2 + ||x||^2$$

or equivalently, the functional

$$\Phi[x;b,\alpha] = ||Tx-b||^2 + \alpha||x||^2 \quad (\alpha>0) . \tag{2.3}$$

When no confusion ensues we will simply refer to this functional as $\Phi[x]$. Note that $\Phi[x]$ is a positive quadratic functional and hence has a unique minimum given by

$$\text{grad } \Phi[x] = 0 .$$

But

$$\text{grad } \Phi[x] = 2T^*(Tx-b) + 2\alpha x$$

and therefore the unique minimum x_α of $\Phi[x]$ is given by

$$x_\alpha = (\tilde{T}+\alpha I)^{-1} T^*b \tag{2.4}$$

(recall that $\tilde{T} := T^*T$). The Tikhonov regularized approximation to the pseudo-normal solution of (1.1) is therefore precisely the minimizer of the functional (2.3). This opens the door for the application of powerful variational techniques in the study of these approximations.

We now present a minor variant of a classical result of Tikhonov [62] which shows that, at least for weak convergence, condition (2.2) on the parameter is not necessary. We shall suppose that $b \in \mathcal{D}(T^\dagger)$ and b^δ satisfies $||Pb-Pb^\delta|| \leq \delta$. This last condition allows b and b^δ to differ by an arbitrarily large component in $R(T)^\perp = N(T^*)$, a reasonable assumption

since any such component is annihilated by T^* in the regularization process. In this regard, note that by "lumping" any component of b which lies in $R(T)^\perp$ into the vector b^δ we may as well assume that $b \in R(T)$, that is, the condition $b \in \mathcal{D}(T^\dagger)$ and $||Pb-Pb^\delta|| \leq \delta$ may always be replaced by $b \in R(T)$ and $||b-Pb^\delta|| \leq \delta$.

Before proving Tikhonov's theorem, we take note of the following simple fact.

Lemma 2.1. For any $b \in Y$, $x_\alpha = (\tilde{T}+\alpha I)^{-1} T^*b \in N(T)^\perp$.

Proposition 2.2. Suppose $b \in \mathcal{D}(T^\dagger)$, $||Pb-Pb^\delta|| \leq \delta$ and that for some positive constants C_1 and C_2, α satisfies $C_1\delta^2 \leq \alpha \leq C_2\delta^2$. Then

$$x_\alpha^\delta \overset{w}{\to} T^\dagger b \quad \text{(weak convergence)}$$

as $\delta \to 0$, where $x_\alpha^\delta = (\tilde{T}+\alpha I)^{-1} T^*b^\delta$.

Proof. Let $x = T^\dagger b$. Since x_α^δ minimizes $\Phi[\cdot;b^\delta,\alpha]$ and

$$\begin{aligned}\Phi[y;b^\delta,\alpha] &= ||Ty-b^\delta||^2 + \alpha||y||^2 \\ &= ||Ty-Pb^\delta||^2 + ||(I-P)b^\delta||^2 + \alpha||y||^2 \\ &= \Phi[y;Pb^\delta,\alpha] + ||(I-P)b^\delta||^2\end{aligned}$$

it follows that x_α^δ minimizes $\Phi[\cdot;Pb^\delta,\alpha]$. Therefore

$$\begin{aligned}&\max\{||Tx_\alpha^\delta-Pb^\delta||^2, C_1\delta^2||x_\alpha^\delta||^2\} \leq \Phi[x_\alpha^\delta;Pb^\delta,\alpha] \\ &\leq \Phi[x;Pb^\delta,\alpha] = ||Tx-Pb^\delta||^2 + \alpha||x||^2 \leq \delta^2 + C_2\delta^2||x||^2 .\end{aligned}$$

It follows that

$$Tx_\alpha^\delta \to Pb \quad \text{as} \quad \delta \to 0 \quad \text{and} \quad \{||x_\alpha^\delta||^2\} \quad \text{is bounded.}$$

For any sequence $\{\delta_n\}$ of positive numbers converging to zero we therefore have a subsequence, again denoted by $\{\delta_n\}$, such that $x_{\alpha_n}^{\delta_n} \overset{w}{\to} u$ for some $u \in X$, where $C_1\delta_n^2 \le \alpha_n \le C_2\delta_n^2$. But since T is weakly continuous, this implies that $Tx_{\alpha_n}^{\delta_n} \overset{w}{\to} Tu$ and hence $Tu = Pb$, i.e. u is a pseudo-solution. Since $x_{\alpha_n}^{\delta_n} \in N(T)^\perp$ for each n (by Lemma 2.1) and since $N(T)^\perp$ is closed and convex (and hence weakly closed), we have $u \in N(T)^\perp$. Therefore $u = x$, the pseudo-normal solution, and for each sequence $\{\delta_n\}$ converging to zero there is a subsequence with $x_{\alpha_n}^{\delta_n} \overset{w}{\to} x$. From this it follows that $x_\alpha^\delta \overset{w}{\to} x$ as $\delta \to 0$. #

The essential features of the argument above, i.e. the use of the variational principle to bound the approximations and then the exploitation of the weak continuity of the operator, will be used several times in the sequel.

It should be remarked that the weak convergence of the regularized approximations may be quite satisfactory if X has a sufficiently strong norm. For example, if we take for X the Sobolev space $W_2^p[a,b]$, being the completion of the space $C^\infty[a,b]$ with respect to the norm

$$||x||^2 = \int_a^b \sum_{i=0}^{p} \left(\frac{d^i x}{dt^i}\right)^2 dt \,,$$

then weak convergence of a sequence of smooth functions implies the uniform convergence of the sequence. The regularized approximations x_α in the space $W_2^p[a,b]$ are called pth order regularized approximations by Tikhonov.

A number of early papers on regularization use a priori choices of the regularization parameter. Tikhonov and Glasko [65] have given a number of illustrations of the use of a choice of the form $\alpha = C\delta^2$ in the numerical solution of integral equations of the first kind by second order regularizors. Franklin [11] suggests the choice $\alpha = \delta^2/\omega^2$ if ω is an a priori bound on the norm of the solution. Ivanov [28] has shown that the condition $\delta = o(\sqrt{\alpha})$ is necessary and sufficient for the strong convergence in L^2 of regularized approximations for Fredholm integral equations of the first kind, while the condition $\delta = O(\sqrt{\alpha})$ is necessary and sufficient for weak convergence in L^2. Khudak [30] shows that if the kernel of the integral operator K is continuous and if the solution lies in $R(K^*)$, then the regularized approximations in L^2 converge uniformly if $\delta = O(\alpha)$. For a positive definite self-adjoint compact operator A, Bakushinskii [4] has studied the "simplified" regularization procedure

$$x_\alpha^\delta = (A+\alpha I)^{-1} b^\delta.$$

If $b \in R(A)$ and $||b-b^\delta|| \leq \delta$, he shows that a sufficient condition for convergence is $\delta = o(\alpha)$ (see also Ivanov [27]

and Khudak [31]). A more general regularization procedure of this type was investigated recently by Franklin [12] from a variational point of view. Finally, we mention that Tikhonov [63] and others have given criteria for an a priori choice of the parameter in the regularization of certain nonlinear problems. In particular, see Ryazantseva [54] and Al'ber [1] for recent results on the regularization of problems involving nonlinear monotone operators.

III. Morozov's Discrepancy Principle

The discrepancy principle of Morozov is based on the reasonable view that the quality of the results of a computation cannot be greater than the quality of the input data. To quote from Morozov [45] "the magnitude of the error must be in agreement with the accuracy of the assignment of the input data of the problem". The discrepancy principle in its simplest form states that if $b \in R(T)$ and $||b-b^{\delta}|| \leq \delta \leq ||b^{\delta}||$, then there is a unique value of the parameter α, which we shall call $\alpha(\delta)$, such that

$$||Tx^{\delta}_{\alpha(\delta)}-b|| = \delta .$$

Here x^{δ}_{α} is the Tikhonov regularized approximation (2.4). Moreover, as $\delta \to 0$, $x^{\delta}_{\alpha(\delta)} \to x$, where x is the normal solution of (1.1). This result, in a slightly altered form, was also published independently by Arcangeli [2] (see also Ivanov [26]) and was to a certain extent implicit in an algorithmic

form in the works of Phillips [53] and Twomey [66].

In this section, we will prove a discrepancy principle under the assumption that $b \in \mathcal{D}(T^\dagger)$ which we have seen is the least we can expect of the data in order to obtain convergence even in the error free case. We shall suppose that $||T||^2 \leq \kappa$ and that the available data consist of a vector $b^\delta \in Y$ satisfying $||Pb-Pb^\delta|| \leq \delta$ (note again that this allows b and b^δ to differ by an arbitrarily large component in $R(T)^\perp$ and therefore we could just as well assume that $b \in R(T)$). Our measure of the "discrepancy" in the approximation is specified by the function

$$\rho(\alpha) := ||\tilde{T}x_\alpha^\delta - T^*b^\delta||^2 .$$

A direct application of Morozov's principle to approximating the pseudo-normal solution would call for monitoring the size of $||Tx_\alpha^\delta - Pb^\delta||$. However, the projection P is not available in the computations which necessitates a slight modification in the method such as the one we now present.

Lemma 3.1. ρ is an increasing continuous function of the positive variable α. Moreover, $\rho(\infty) = ||T^*b^\delta||^2$ and $\rho(0) = 0$.

Proof. First note that $x_\infty^\delta = 0$ and hence $\rho(\infty) = ||T^*b^\delta||^2$. If we denote the spectral resolution of the positive self-adjoint operator $\tilde{T}$ by $\{E_\lambda\}$, then we have the representation

$$\rho(\alpha) = \int_{0-}^{||T||^2} \left(\frac{\alpha}{\lambda+\alpha}\right)^2 d\,||E_\lambda T^*b^\delta||^2 ,$$

from which it follows that ρ is increasing and continuous. Also, $\rho(0) = ||P_{N(T)}\, T^*b^\delta||^2 = 0$ since $T^*b^\delta \in N(T)^\perp$. #

Note that if y is any pseudo-solution then

$$||\tilde{T}y - T^*b^\delta||^2 = ||T^*Pb - T^*Pb^\delta||^2 \leq \kappa\delta^2 . \qquad (3.1)$$

Moreover, a vector z of minimal norm satisfying the above inequality also satisfies

$$||\tilde{T}z - T^*b^\delta||^2 = \kappa\delta^2$$

for if

$$a := ||\tilde{T}z - T^*b^\delta|| < \kappa^{1/2}\delta \quad \text{and} \quad \gamma = \min\left\{1, \frac{\kappa^{1/2}\delta - a}{\kappa||z||}\right\}$$

then the vector $y = (1-\gamma)z$ has norm smaller than $||z||$ and satisfies (3.1). This suggests considering the regularized approximations

$$x_\alpha^\delta = (\tilde{T}+\alpha I)^{-1} T^*b^\delta$$

where the parameter α is chosen according to the condition

$$\rho(\alpha) = ||\tilde{T}x_\alpha^\delta - T^*b^\delta||^2 = \kappa\delta^2 . \qquad (3.2)$$

From the lemma it follows that if $\kappa\delta^2 \leq ||T^*b^\delta||^2$, then there is a unique number $\alpha(\delta)$ satisfying $\rho(\alpha(\delta)) = \kappa\delta^2$.

The following result shows that this choice of the parameter, which relates the discrepancy in the approximation to the level of error in the input data, gives a stable approximation scheme for computing the pseudo-normal solution.

Proposition 3.2. Suppose $b \in \mathcal{D}(T^\dagger)$, $||Pb-Pb^\delta|| \leq \delta$ and $\kappa\delta^2 \leq ||T^*b^\delta||^2$ where $||T||^2 \leq \kappa$, then $x^\delta_{\alpha(\delta)} \to T^\dagger b$ as $\delta \to 0$ if $\rho(\alpha(\delta)) = \kappa\delta^2$.

Proof. We first recall that the Tikhonov approximation $x_\alpha = (\tilde{T}+\alpha I)^{-1}T^*y$ minimizes the functional Φ defined by

$$\Phi[z;Py,\alpha] = ||Tz-Py||^2 + \alpha||z||^2 .$$

Therefore, if $x = T^\dagger b$, then

$$\Phi[x^\delta_{\alpha(\delta)};Pb^\delta,\alpha(\delta)] \leq \Phi[x;Pb^\delta,\alpha(\delta)] ,$$

and hence

$$||Tx^\delta_{\alpha(\delta)}-Pb^\delta||^2 + \alpha(\delta)||x^\delta_{\alpha(\delta)}||^2 \leq ||Tx-Pb^\delta||^2 + \alpha(\delta)||x||^2$$
$$= ||Pb-Pb^\delta||^2 + \alpha(\delta)||x||^2 \leq \delta^2 + \alpha(\delta)||x||^2 .$$

However,

$$||Tx^\delta_{\alpha(\delta)}-Pb^\delta||^2 \geq \kappa^{-1}||T||^2||Tx^\delta_{\alpha(\delta)}-Pb^\delta||^2$$
$$\geq \kappa^{-1}||\tilde{T}x^\delta_{\alpha(\delta)}-T^*b^\delta||^2 = \kappa^{-1}\rho(\alpha(\delta)) = \delta^2 .$$

Substituting this in the inequality above, we have

$$||x^\delta_{\alpha(\delta)}|| \leq ||x|| \qquad (3.3)$$

for all $\delta > 0$. Therefore the set $\{x^{\delta}_{\alpha(\delta)}:\delta>0\}$ is bounded and hence weakly pre-compact.

Suppose now that $\{\delta_n\}$ is any sequence of positive numbers converging to zero. Then there is a subsequence, again denoted by $\{\delta_n\}$, with $x^{\delta_n}_{\alpha(\delta_n)} \overset{w}{\to} y$. Also,

$$\begin{aligned}||\tilde{T}x^{\delta_n}_{\alpha(\delta_n)}-\tilde{T}x|| &\le ||\tilde{T}x^{\delta_n}_{\alpha(\delta_n)}-T^*b^{\delta_n}|| + ||T^*b^{\delta_n}-\tilde{T}x|| \\ &= \kappa^{1/2}\delta_n + ||T^*b^{\delta_n}-T^*b|| \\ &= \kappa^{1/2}\delta_n + ||T^*P(b^{\delta_n}-b)|| \\ &\le 2\kappa^{1/2}\delta_n \to 0 \quad \text{as} \quad n \to \infty .\end{aligned}$$

Therefore $x^{\delta_n}_{\alpha(\delta_n)} \overset{w}{\to} y$ and $\tilde{T}x^{\delta_n}_{\alpha(\delta_n)} \to \tilde{T}x$ as $n \to \infty$. It now follows as in proof of Proposition 2.2 that $y = x$ and

$$x^{\delta}_{\alpha(\delta)} \overset{w}{\to} x \quad \text{as} \quad \delta \to 0. \tag{3.4}$$

For any convergent sequence $\{||x^{\delta_n}_{\alpha(\delta_n)}||\}$ we have

$$||x||^2 = \lim_{n\to\infty} |\langle x, x^{\delta_n}_{\alpha(\delta_n)}\rangle| \le ||x|| \lim_{n\to\infty} ||x^{\delta_n}_{\alpha(\delta_n)}||$$

and therefore

$$||x|| \le \liminf_{\delta \to 0} ||x^{\delta}_{\alpha(\delta)}|| .$$

But by (3.3)

$$\limsup_{\delta \to 0} ||x^{\delta}_{\alpha(\delta)}|| \le ||x||$$

and hence $||x|| = \lim_{\delta\to 0} ||x^{\delta}_{\alpha(\delta)}||$. This combined with (3.4) proves that

$$\lim_{\delta \to 0} x^{\delta}_{\alpha(\delta)} = x. \quad \#$$

In using the discrepancy method it would be helpful to have an a priori bound on the regularization parameter. Vinokorov [67] has provided such a bound. A slight modification of Vinokorov's argument yields the following result.

Proposition 3.3. If the parameter α is chosen according to criterion (3.2) above, then

$$\alpha \leq \kappa^{3/2} \delta / (||T^* b^{\delta}||^2 - \kappa^{1/2} \delta) .$$

We have considered the discrepancy method only in a very simple context but we wish to point out that the method has been highly developed by Morozov and his colleagues (see the works of Morozov and Goncharskii et al. in the references).

IV. OTHER A POSTERIORI METHODS

The discrepancy method is but one of a number of a posteriori strategies which have been proposed for choosing the regularization parameter. In order to motivate some of these methods we recall some facts about the accuracy in Tikhonov regularization. It is well known that if $Pb \in R(TT^*)$ then the (error-free) Tikhonov method converges with a rate $\alpha^{1/2}$ (see e.g. [29]). However, if the data satisfy stronger assumptions methods can be devised with a corresponding higher rate of convergence (see [21] for a general result along these lines).

In particular what we might recall the iterated Tikhonov method given by

$$z_\alpha := \alpha(\tilde{T}+\alpha I)^{-1}x_\alpha + x_\alpha$$

where

$$x_\alpha := (\tilde{T}+\alpha I)^{-1}T^*b$$

has been investigated by Dorofeev [9] and King and Chillingworth [32]. If $Pb \in R(TT^*T)$ then it can be shown that z_α converges with a rate $\alpha^{3/2}$ [32]. Note that

$$\frac{dx_\alpha}{d\alpha} = -(\tilde{T}+\alpha I)^{-2}T^*b = -(\tilde{T}+\alpha I)^{-1}x_\alpha$$

and hence

$$\alpha\frac{dx_\alpha}{d\alpha} = -\alpha(\tilde{T}+\alpha I)^{-1}x_\alpha = x_\alpha - z_\alpha .$$

Therefore a choice of α which minimizes

$$\left|\left|\alpha\frac{dx_\alpha}{d\alpha}\right|\right| \qquad (4.1)$$

tends to move the "cheap" approximation x_α closer to the generally more accurate approximation z_α. In the presence of erroneous data a value of α which minimizes (4.1) is called in the Soviet literature a quasi-optimal choice of the parameter ([64],[65]), but we shall call it a choice by the <u>derivative criterion</u>. For a numerical example of the use of this parameter choice criterion in an inverse problem in heat conduction, see

Glasko et al. [13].

Another approach, Tikhonov and Arsenin's ratio criterion, in our context advocates maximizing the ratio

$$||\tilde{T}z_\alpha^\delta - T^*b^\delta||/||\tilde{T}x_\alpha^\delta - T^*b^\delta|| ,$$

which tends to make the residual of x_α^δ as small as possible relative to the residual of z_α^δ.

We now present some arguments of Leonov [38] who has established the convergence of the simplified Tikhonov method in finite dimensional space using the derivative criterion for the choice of the parameter. We shall therefore assume that $T : \mathbb{R}^m \to \mathbb{R}^n$ is linear. Then the pseudo-solutions of equation

$$Tx = b$$

are the solutions of

$$Ax = y \tag{4.2}$$

where $A = T^*T$ is an n by n symmetric matrix and $y = T^*b \in N(A)^\perp = R(A)$. We assume a vector $y^\delta \in \mathbb{R}^n$ is on hand satisfying $||y-y^\delta|| \leq \delta$ (Euclidean norm) and we seek to approximate the normal solution of (4.2) by the simplified Tikhonov approximation

$$x_\alpha^\delta := (A+\alpha I)^{-1}y^\delta =: U_\alpha(A)y^\delta .$$

The ideal simplified Tikhonov approximation will be denoted by

x_α, viz.

$$x_\alpha := (A+\alpha I)^{-1}y = U_\alpha(A)y \ .$$

Suppose that $0 < \lambda_1 \le \lambda_2 \le \ldots \le \lambda_r$ is the complete system of positive eigenvalues of A and $\{u_k\}_{k=1}^r$ is a corresponding system of orthonormal eigenvectors. Since $y \in R(A) = N(A)^\perp$ we have a representation of the form

$$y = \sum_{k=1}^{r} a_k u_k \ .$$

Also, for suitable coefficients $\{a_k^\delta\}$ we have

$$y^\delta = w^\delta + \sum_{k=1}^{r} a_k^\delta u_k$$

where $w^\delta \in N(A)$. We therefore have

$$\delta^2 \ge ||y-y^\delta||^2 = ||w^\delta||^2 + \sum_{k=1}^{r} (a_k-a_k^\delta)^2 \ge ||w^\delta||^2 \ . \quad (4.3)$$

We now set

$$F(\alpha) := \left|\left|\alpha \frac{dx_\alpha^\delta}{d\alpha}\right|\right|^2$$

$$= ||\alpha U_\alpha(A)^2 y^\delta||^2$$

$$= ||w^\delta||^2/\alpha^2 + \alpha^2 \sum_{k=1}^{r} (a_k^\delta)^2/(\alpha+\lambda_k)^4 \ .$$

A little calculus shows that F has a smallest relative minimum which we denote by α' (the choice of α by the derivative criterion). From the fact that $F'(\alpha') = 0$ one obtains

$$||w^\delta||^2/\alpha'^4 = 2 \sum_{k=1}^{r} \left\{1 - \frac{2\alpha'}{\alpha'+\lambda_k}\right\} (a_k^\delta)^2/(\alpha'+\lambda_k)^4 \qquad (4.4)$$
$$\leq 2 \sum_{k=1}^{r} (a_k^\delta)^2/\lambda_k^4$$

and therefore $||w^\delta||^2/\alpha'^4$ is bounded for small δ. Moreover the equality above shows that α' is bounded as $\delta \to 0$, for otherwise the left hand side would become negative for small δ. If we suppose that $\alpha' \leq m$, then

$$\sum_{k=1}^{r} \left\{1 - \frac{2\alpha'}{\alpha'+\lambda_k}\right\} (a_k^\delta)^2/(\alpha'+\lambda_k)^4 \geq \sum_{k=1}^{r} \left\{1 - \frac{2m}{m+\lambda_k}\right\}$$
$$(a_k^\delta)^2/(m+\lambda_k)^4 .$$

Since $a_k^\delta \to a_k$ as $\delta \to 0$, it follows from (4.4) that for δ sufficiently small

$$\delta^2 \geq ||w^\delta||^2 \geq C\alpha'^4$$

for some positive constant C and hence $\alpha' \to 0$ as $\delta \to 0$.

To establish the convergence of $x_{\alpha'}^\delta$ to the normal solution x we note that

$$||x_{\alpha'}^\delta - x|| \leq ||x_{\alpha'}^\delta - x_{\alpha'}|| + ||x_{\alpha'} - x|| .$$

But it is well known that in the absense of error in the right hand side the simplified Tikhonov method converges to the normal solution. Since $\alpha' \to 0$ as $\delta \to 0$ we therefore have $||x_{\alpha'} - x|| \to 0$ as $\delta \to 0$. Therefore, we need only estimate the quantity $||x_{\alpha'}^\delta - x_{\alpha'}||$. To this end, we give the following

lemma.

Lemma 4.1. $||x_\alpha^\delta - x_\alpha|| \le ||w^\delta||/\alpha + \delta/\lambda_1$.

Proof. Note that

$$x_\alpha^\delta - x_\alpha = U_\alpha(A)(y^\delta - y) = U_\alpha(A)\left[w^\delta + \sum_{k=1}^{r} (a_k^\delta - a_k)u_k\right]$$

$$= U_\alpha(A)\ (w^\delta + Az^\delta)$$

where

$$z^\delta = \sum_{k=1}^{r} (a_k^\delta - a_k)u_k/\lambda_k \ .$$

But by (4.3),

$$||z^\delta||^2 = \sum_{k=1}^{r} (a_k^\delta - a_k)^2/\lambda_k^2 \le \lambda_1^{-2} \sum_{k=1}^{r} (a_k^\delta - a_k)^2 \le (\lambda_1^{-1}\delta)^2 \ .$$

Since $||U_\alpha(A)|| \le \alpha^{-1}$ and $||AU_\alpha(A)|| \le 1$ we then have

$$||x_\alpha^\delta - x_\alpha||^2 = \langle x_\alpha^\delta - x_\alpha, U_\alpha(A)w^\delta \rangle + \langle x_\alpha^\delta - x_\alpha, AU_\alpha(A)z^\delta \rangle$$

$$\le ||x_\alpha^\delta - x_\alpha|| \ [||w^\delta||/\alpha + \delta/\lambda_1] \ . \quad \#$$

Finally, for the choice $\alpha = \alpha'$ we have seen that there is a constant, say C_1, such that $C_1||w^\delta||^{1/2} \le \alpha'$ for δ sufficiently small. Substituting this in the lemma and using (4.3) we have

$$||x_{\alpha'}^\delta - x_{\alpha'}|| \le \sqrt{\delta}/C_1 + \delta/\lambda_1 \to 0 \quad \text{as} \quad \delta \to 0,$$

which proves:

Proposition 4.2. In the case of simplified Tikhonov regulariza-

tion in a finite dimensional space the choice of parameter by the derivative criterion gives a method which converges to the normal solution.

The choice of the regularization parameter by the derivative criterion is related to a method for selecting the regularization parameter investigated by Hilgers [24]. He notes that the optimal value of the regularization parameter is a value which minimizes the function

$$e(\alpha) = ||x_\alpha^\delta - T^\dagger b||^2 .$$

Differentiating this with respect to α we have

$$e'(\alpha)/2 = \langle x_\alpha^\delta - T^\dagger b, \frac{dx_\alpha^\delta}{d\alpha} \rangle .$$

Therefore, the optimal value of the parameter, α_0, should satisfy

$$\langle x_{\alpha_0}^\delta - T^\dagger b, \left.\frac{dx_\alpha^\delta}{d\alpha}\right|_{\alpha=\alpha_0} \rangle = 0 . \tag{4.5}$$

If we assume that we have a genuinely ill-posed problem then $\alpha_0 > 0$ and this condition is equivalent to

$$\langle x_{\alpha_0}^\delta - T^\dagger b, \alpha \left.\frac{dx_\alpha^\delta}{d\alpha}\right|_{\alpha=\alpha_0} \rangle = 0 .$$

Since

$$\langle x_\alpha^\delta - T^\dagger b, \alpha \frac{dx_\alpha^\delta}{d_\alpha} \rangle \leq ||x_\alpha^\delta - T^\dagger b||\ ||\alpha \frac{dx_\alpha^\delta}{d\alpha}|| ,$$

we may view the derivative criterion as an attempt to approximately satisfy (4.5). Hilgers takes a different tack. Since $TT^{\dagger}b = Pb$ and

$$\frac{dx_{\alpha}^{\delta}}{d\alpha} = -U_{\alpha}(\tilde{T})^2 T^* b^{\delta} = -T^* U_{\alpha}(\hat{T})^2 b^{\delta} ,$$

where $\hat{T} := TT^*$, he writes (4.5) as

$$\langle Pb - Tx_{\alpha_0}^{\delta}, U_{\alpha_0}(\hat{T})^2 b^{\delta} \rangle = 0. \tag{4.6}$$

All of the quantities on the left are computable except for the projection Pb. But if $b \in \overline{R(T)}$ (or if T is self-adjoint and one-to-one) then $Pb = b$ and (4.6) becomes

$$\langle b - Tx_{\alpha_0}^{\delta}, U_{\alpha_0}(\hat{T})^2 b^{\delta} \rangle = 0 .$$

But of course the vector b is also unavailable and therefore Hilgers advocates a choice of α which minimizes the expression

$$\langle b^{\delta} - Tx_{\alpha}^{\delta}, U_{\alpha}(\hat{T})^2 b^{\delta} \rangle .$$

Note that this quantity is nonnegative because

$$\begin{aligned} b^{\delta} - Tx_{\alpha}^{\delta} &= (I - TU_{\alpha}(\tilde{T})T^*)b^{\delta} \\ &= (I - \hat{T}U_{\alpha}(\hat{T}))b^{\delta} \\ &= \alpha U_{\alpha}(\hat{T})b^{\delta} \end{aligned}$$

and therefore

$$\langle b^{\delta} - Tx_{\alpha}^{\delta}, U_{\alpha}(\hat{T})^2 b^{\delta} \rangle = \alpha \langle U_{\alpha}(\hat{T})b^{\delta}, U_{\alpha}(\hat{T})^2 b^{\delta} \rangle = \alpha \| U_{\alpha}(\hat{T})^{3/2} b^{\delta} \|^2 .$$

We might also notice that this equality also gives the bound

$$\langle b^\delta - Tx_\alpha^\delta, U_\alpha(\hat{T})^2 b^\delta \rangle \leq (||b^\delta||/\alpha)^2$$

since $||U_\alpha(\hat{T})|| \leq \alpha^{-1}$. The use of this method of choosing the parameter has been tested on sample problems in [23] and [24]. It should be remarked that the choice of the parameter by Hilger's criterion requires an additional inversion as $U_\alpha(\hat{T})$ is not obtainable directly from $U_\alpha(\tilde{T})$.

One can also verify the convergence of simplified Tikhonov regularization in a finite dimensional space with Hilger's choice of the parameter. The essential point is to find an upper bound for $||w^\delta||$ in terms of the parameter and use Lemma (4.1). To this end, we will use the notation established above in the discussion of the simplified regularization method for the equation $Ax = y$.

We will denote by α_n a value of α which minimizes the function

$$F(\alpha) = \alpha \langle U_\alpha(A) y^\delta, U_\alpha(A)^2 y^\delta \rangle$$

$$= ||w^\delta||^2/\alpha + \alpha \sum_{k=1}^{r} (a_k^\delta)^2/(\alpha+\lambda_k)^3 .$$

Using $F'(\alpha_h) = 0$, we find that

$$2||w^\delta||^2/\alpha_h^3 \leq \sum_{k=1}^{r} (a_k^\delta)^2/\lambda_k^3 .$$

Therefore for δ sufficiently small, we have $\alpha_h \geq C_2 ||w^\delta||^{2/3}$ for some positive constant C_2. As in the proof of Proposition

4.2 we may now conclude that

$$x_{\alpha_h}^{\delta} \to x \quad \text{as} \quad \delta \to 0 \ .$$

V. IVANOV'S CONSTRAINED PSEUDO-SOLUTIONS

Ivanov and his colleagues ([25],[8]) have studied generalized solutions of the linear operator equation

$$Tx = b \tag{5.1}$$

which are required to satisfy a certain norm constraint (see also Miller's [41] "method 4"). In studying the parameter choice problem for a regularized approximation to such a generalized solution we shall employ terminology and notation which is more consistent with that which we have used in the previous sections rather than adhering to that used by Ivanov.

We suppose that T is a bounded linear operator from a Hilbert space X into a Hilbert space Y and that R is a fixed positive number. The closed ball in X of radius R will be denoted by B_R, i.e. $B_R = \{x \in X: ||x|| \leq R\}$. By an R-pseudo-solution of (5.1) we mean a vector $x \in B_R$ satisfying

$$||Tx-b|| = \inf \{||Tz-b|| : z \in B_R\} \ .$$

We note that an R-pseudo-solution always exists since B_R is weakly compact and the functional $f(z) = ||Tz-b||$ is weakly lower semicontinuous. It is useful to characterize the set of R-pseudo-solutions in a more geometrical way. First note that

the set TB_R is weakly closed and convex and therefore strongly closed. If we denote by Q the metric projection of Y onto TB_R, that is if Qy is the unique element of TB_R which is nearest to $y \in Y$, then Q is continuous. It follows directly from the definition that x is an R-pseudo-solution of (5.1) if and only if

$$Tx = Qb.$$

If we denote the set of all R-pseudo-solutions by X_R, i.e.

$$X_R = \{x \in B_R : Tx = Qb\},$$

then X_R is closed, convex and nonempty. The set X_R therefore has a unique element of smallest norm which we will denote by x_R and call the R-pseudo-normal solution of (5.1). The term normal is used since

$$X_R \cap N(T)^{\perp} = \{x_R\}.$$

Indeed, if $u \in X_R$ and $u = u_1 + u_2 \in N(T) \oplus N(T)^{\perp}$, then since $||u||^2 = ||u_1||^2 + ||u_2||^2$ we see that $u_2 \in B_R$ and moreover $Tu_2 = Tu = Qb$. Furthermore $||u||^2$ is minimal if and only if $u_1 = 0$, i.e. $u \in N(T)^{\perp}$.

Note that if equation (5.1) has a pseudo-solution, that is if $b \in \mathcal{D}(T^{\dagger})$, then $x_R = T^{\dagger}b$ if and only if $||T^{\dagger}b|| \leq R$.

Lemma 5.1. If $||T^{\dagger}b|| > R$, then $||x_R|| = R$.

Proof. First note that $b \neq Qb$. For if $Qb = b$ then $b = Tx$

for some $x \in B_R$ and hence

$$b = Pb = Tx .$$

Therefore x is a pseudo-solution and hence

$$R < ||T^\dagger b|| \leq ||x|| \leq R .$$

Suppose that $||b-Qb|| = \gamma > 0$ and

$$S_\gamma := \{y \in Y : ||y-b|| \leq \gamma\} .$$

Then

$$S_\gamma \cap TB_R = \{Qb\} ,$$

each of S_γ and TB_R is convex, and S_γ has an interior. Therefore by the Hahn-Banach separation theorem there is a linear functional ϕ such that $\phi(y) \leq 1$ for $y \in TB_R$ and $\phi(y) \geq 1$ for $y \in S_\gamma$. If $||x_R|| < R$ then there is a $\beta > 1$ such that $\beta x_R \in B_R$. We then have

$$1 < \beta = \beta\phi(Qb) = \beta\phi(Tx_R) = \phi(T_\beta x_R) \leq 1. \quad \#$$

Lemma 5.2. The functional $g(z) = ||T^\dagger z||$ is lower semi-continuous on $\mathcal{D}(T^\dagger)$.

Proof. Suppose $\{y_n\} \subset \mathcal{D}(T^\dagger)$, $y_n \to y$ and $||T^\dagger y_n|| \leq m$. Then there is a subsequence $\{y_{n_k}\}$ and a $z \in X$ with

$$T^\dagger y_{n_k} \overset{w}{\to} z .$$

Since B_m is weakly closed we have $||z|| \leq m$. Since $T^\dagger$ is a closed linear operator, it is also weakly closed. But $y_{n_k} \overset{w}{\to} y$ and $T^\dagger y_{n_k} \overset{w}{\to} z$ then implies that $y \in \mathcal{D}(T^\dagger)$ and $T^\dagger y = z$. Therefore $||T^\dagger y|| \leq m$. #

Lemma 5.3. Suppose $b \in \mathcal{D}(T^\dagger)$ and $||T^\dagger b|| > R$. If $||Pb-Pb^\delta|| \leq \delta$, then for all sufficiently small δ there is a unique $\alpha = \alpha(\delta)$ such that $||x^\delta_{\alpha(\delta)}|| = R$ where $x^\delta_\alpha = (\bar{T}+\alpha I)^{-1}T^*b^\delta$.

Proof. It is not difficult to see that the function $g(\alpha) := ||x^\delta_\alpha||$ is continuous, decreasing and satisfies $g(\infty) = 0$. If $b^\delta \notin \mathcal{D}(T^\dagger)$ then $g(0) = \infty$ (see the introduction). While if $b^\delta \in \mathcal{D}(T^\dagger)$ then $g(0) = ||T^\dagger b^\delta|| = ||T^\dagger Pb^\delta|| > R$ for δ sufficiently small by Lemma 5.2. The result now follows. #

Proposition 5.4. If $b \in \mathcal{D}(T^\dagger)$, $||T^\dagger b|| > R$ and $||Pb-Pb^\delta|| \leq \delta$, then

$$\lim_{\delta \to 0} x^\delta_{\alpha(\delta)} = x_R .$$

Proof. Since x^δ_α minimizes the functional

$$\Phi[x;b^\delta,\alpha] = ||Tx-b^\delta||^2 + \alpha||x||^2$$

we have $\Phi[x^\delta_\alpha;b^\delta,\alpha] \leq \Phi[x_R;b^\delta,\alpha]$, that is,

$$||Tx^\delta_\alpha-b^\delta||^2 + \alpha||x^\delta_\alpha||^2 \leq ||Tx_R-b^\delta||^2 + \alpha R^2 .$$

For the choice $\alpha = \alpha(\delta)$ we have $||x^{\delta}_{\alpha(\delta)}||^2 = R^2$ and hence

$$||Tx^{\delta}_{\alpha(\delta)}-b^{\delta}||^2 \leq ||Tx_R-b^{\delta}||^2 = ||Qb-b^{\delta}||^2 \to ||Qb-b||^2 \text{ as } \delta \to 0 .$$

Therefore

$$\limsup_{\delta \to 0} ||Tx^{\delta}_{\alpha(\delta)}-b^{\delta}|| \leq ||Qb-b|| .$$

Since $\{||x^{\delta}_{\alpha(\delta)}||\}$ is bounded, for any sequence $\{\delta_n\}$ of positive numbers converging to zero there is a subsequence, again denoted by $\{\delta_n\}$ such that $x^{\delta_n}_{\alpha(\delta_n)} \overset{w}{\to} x$. We may conclude as in previous proofs that $x \in N(T)^{\perp} \cap B_R$ and $Tx^{\delta_n}_{\alpha(\delta_n)} \overset{w}{\to} Tx$. Now if $z \in Y$ and $||z|| = 1$, we have

$$|\langle Tx-b,z\rangle| = \lim_n |\langle Tx^{\delta_n}_{\alpha(\delta_n)}-b,z\rangle| \leq ||Qb-b|| .$$

Therefore $||Tx-b|| \leq ||Qb-b||$ and hence $Tx = Qb$, i.e.

$$x \in X_R \cap N(T)^{\perp} = \{x_R\} .$$

We now have $x^{\delta}_{\alpha(\delta)} \overset{w}{\to} x_R$ as $\delta \to 0$ and $||x^{\delta}_{\alpha(\delta)}|| = R = ||x_R||$ and hence

$$x^{\delta}_{\alpha(\delta)} \to x_R \text{ as } \delta \to 0 . \quad \#$$

The result above gives a parameter choice criterion for approximating the R-pseudo-normal solution assuming some a priori information on the pseudo-normal solution, namely that its norm is greater than R. If the pseudo-normal solution has norm

less than or equal to R then the R-pseudo-normal solution coincides with the pseudo-normal solution and any of the parameter choice criteria from the previous sections may be used in computing the regularized approximations.

VII. CONCLUDING REMARKS

The mathematical theory of regularization for linear ill-posed problems has developed very rapidly and in many directions during the past seventeen years. Our presentation of the parameter choice problem was rather narrowly aimed and in this section we wish to take our last opportunity to briefly mention some related topics.

The parameter choice criteria presented above are theoretical in that they do not indicate how the parameter is chosen in actual computational practice. One rough and ready way to choose the parameter in practice is to perform a regularization for several values of the parameter, say α, $\alpha/10$, $\alpha/10^2$, ... where α is fixed (and not "too small"). One then takes the value of the parameter which comes closest to satisfying the chosen criterion. This has been called the "selection" method. Gordonova and Morozov [19] (see also [18]) have investigated the use of Newton's method as a more sophisticated procedure for solving numerically for the chosen regularization parameter.

The point has been made above that the great analytical success of Tikhonov's method is due in large measure to its simple variational interpretation. There are other types of

regularization methods, for example iterative methods ([34], [35], [39]) in which the role of the regularization parameter is played by a discrete parameter (e.g. the iteration number) and for which there is no natural variational interpretation. There seems to be no satisfactory parameter choice criterion for such methods. Ill-posed problems may also be regularized by the use of expansion methods ([3], [37], [55]) or finite element type methods ([51], [68], [40]) which also depend on a discrete parameter (the dimension of a subspace).

We have taken a purely deterministic point of view in this presentation but there is a substantial literature on regularization in which statistical properties of an error distribution are assumed and corresponding stochastic convergence properties of the regularized approximations are derived. We refer the reader to [7], [10], [46] and [59] for details and references.

Finally, we mention that Strahov and his colleagues [56], [57], [58] have studied a somewhat more general linear ill-posed problem than the one we considered above. Namely, they study the problem of constructing the values of a closed unbounded operator. Since the generalized inverse is in general closed and unbounded their results apply in our context.

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Department of Mathematical Sciences
University of Cincinnati
Cincinnati, Ohio 45221

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