PROJECTION-REGULARIZATION METHODS FOR LINEAR OPERATOR EQUATIONS OF THE FIRST KIND*

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1. Introduction

We review some basic facts about linear operator equations of the first kind. For details and references see e.g. [8].

Many inverse problems of mathematical physics, as well as problems of indirect measurement or remote sensing, are modeled by Fredholm integral equations of the first kind, that is, equations of the form

$$\int_a^b k(s,t)x(t)dt = y(s), \tag{1}$$

where $k(.,.)$ is a given kernel and y is a given function called the "data". A Fredholm integral equation of the first kind can be phrased abstractly as

$$Kx = y \tag{2}$$

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where $K:H_1 \to H_2$ is bounded linear operator from a real Hilbert space H_1 into a real Hilbert space H_2 (the symbols $(.,.)$ and $\|.\|$ will be used to denote the inner product and norm, respectively, in each of the spaces H_1 and H_2 and also in $\mathbb{R}^n$; whenever there is a danger of confusion we specifically indicate which norm is meant by writing e.g. $\|.\|_{\mathbb{R}^n}$).

It is well known that equations of the type (2) are generally ill-posed, that is, a solution does not always exist, when solutions exist they are not generally unique, and, when a unique solution exists it does not necessarily depend continuously on the data y. When a solution in the traditional sense does not exist one can seek a <u>least squares solution</u>, that is, a vector x satisfying

$$\| Kx - y\| = \inf\{ \|Ku - y\|: u \in H_1 \}.$$

This is equivalent to

$$K^*Kx = K^*y \tag{3}$$

where K^* is the adjoint of the operator K. Least squares solutions are generally not unique, however, the set of least squares solutions is closed and convex and hence contains a unique vector of smallest norm. The unique minimal norm least squares solution of (2) is denoted by $K^\dagger y$, where the operator $K^\dagger: D(K^\dagger) \to H_1$ is called the <u>Moore-Penrose generalized inverse</u> of the operator K. It is not difficult to show that $K^\dagger$ is closed linear operator with dense domain $D(K^\dagger)=R(K)\dot{+}R(K)^\perp$, where R(K) is the range of K. The major difficulty in the practical solution of (3) arises from the fact that the generalized solution operator $K^\dagger$ is discontinuous if (2) is ill-posed.

In many applications (e.g., if (2) is induced by (1) with an L^2-kernel k) the operator K is compact and in this case $K^\dagger$ is continuous if and only if R(K) is finite dimensional, that is, if and only if the kernel k in (1) is degenerate. Therefore the generalized existence and uniqueness formalism provided by the generalized inverse operator does not, except in trivial instances, impose continuity on the solution process.

The essential discontinuity of the generalized solution operator has dire consequences when solving practical Fredholm equations of the first kind. In such problems the data function y is not known precisely, but rather is the result of measurements. The function y is therefore an idealization and the actual data is a function y^δ that approximates y in the sense that $\|y - y^\delta\| \leq \delta$, where δ is a known error level that depends upon the quality of the measurement process. Instead of this bound on the norm of the error, one might also have statistical information on the error.

Since the equation (3) is ill-posed, any attempt to solve it using erroneous data y^δ instead of the exact data y can lead to large deviations in the computed solution due to the discontinuous nature of the generalized solution operator $K^\dagger$. The instability inherent in solving (3) can be mitigated by replacing (3) with a nearby well-posed problem. We describe a very general way of doing this.

If the operator K^*K is invertible, then the solution of (3) may be written as $x = (K^*K)^{-1}K^*y$. However, whenever $K^\dagger$ is unbounded (and not only then) K^*K has no bounded inverse. The idea is to approximate x by

$$x_\alpha = U_\alpha(K^*K)K^*y \tag{4}$$

where $U_\alpha(\lambda)$ is a continuous function on $[0, \|K\|^2]$ which approximates λ^{-1} in an appropriate sense.

Specifically we assume that for some constant C

$$|\lambda U_\alpha(\lambda)| \leq C \text{ and } U_\alpha(\lambda) \to \lambda^{-1} \text{ as } \alpha \to 0$$

for each $\lambda \in]0, \|K\|^2]$. The essential points are that x_α defined by (4) depends continuously on y for each fixed $\alpha > 0$ and that $x_\alpha \to K^\dagger y$ as $\alpha \to 0$ if (and only if) $y \in D(K^\dagger)$. The approximations (4) therefore provide well-posed estimates of the minimal norm least squares solution of (2). Moreover, it is not difficult to derive order of convergence estimates for $\|x - x_\alpha\|$ based on properties of the function $U_\alpha(\lambda)$ and generalized smoothness or regularity conditions on the minimal norm least squares solution x.

As pointed out above, a significant practical difficulty arises from the fact that the exact data y is unknown and only an approximation y^δ to the data satisfying $\|y - y^\delta\| \leq \delta$ is available. One must then work with the approximations

$$x_\alpha^\delta = U_\alpha(K^*K)K^*y^\delta \tag{5}$$

which use the available approximate data y^δ. This scheme is said to constitute a regularization method if there is a choice $\alpha = \alpha(\delta)$ of the regularization parameter such that $x_{\alpha(\delta)}^\delta \to K^\dagger y$ as $\delta \to 0$ (see [8], [10], [13] for surveys of ill-posed problems and regularization methods).

It is not difficult to show that

$$\|x_\alpha - x_\alpha^\delta\| \leq \delta \sqrt{Cg(\alpha)}$$

where $g(\alpha) = \max\{|U_\alpha(\lambda)| : \lambda \in [0, \|K\|^2]\}$, and hence $\delta\sqrt{g(\alpha)} \to 0$ is a general sufficient condition for the regularity of (4).

Note that this estimate could be replaced by

$$\|x_\alpha - x_\alpha^\delta\| \leq \delta . h(\alpha)$$

with $h(\alpha)^2 := \max\{|\lambda U_\alpha(\lambda)^2| : \lambda \in [0, \|K\|^2]\}$ (cf. [1]), which is a sharper estimate if the spectrum of K^*K decays faster than exponentially (cf. [6]). We work with the first estimate here, although in the

case mentioned one could obtain slightly better results using the second estimate in an analogous way.

It must be kept in mind, that the asymptotic theory of regularization briefly outlined above involves approximations x_α^δ which are not effectively computable since the operators K^*K and K^* act on infinite dimensional spaces. Effectively computable approximations are obtained by working in a finite dimensional subspace and would involve the introduction of a new regularization parameter, the dimension of the subspace.

A number of authors ([5],[9],[14],[17]) have studied finite dimensional approximations obtained by projecting regularized approximations into finite dimensional subspaces. Such methods may be called regularization-projection methods.

Also, a number of papers (e.g. [3],[4],[16]) deal with regularization by projection, where the projection into finite dimensional subspaces acts as regularization without additional regularization in the infinite dimensional setting.

In this note we will consider projection-regularization methods, that is, methods obtained by projecting the operator first and then applying a regularization method.

We will illustrate the difference between regularization-projection methods and projection-regularization methods in Section 3.

2. Projection-Regularization Methods

Suppose that $\{v_1, v_2, \ldots, v_n\}$ are linearly independent vectors in $\overline{R(K)}$ such that $\bigcup_{n=1}^{\infty} \text{span}\{v_1, v_2, \ldots v_n\}$ is dense in $\overline{R(K)}$. Define an

operator $r_n: H_2 \to \mathbb{R}^n$ by

$$r_n y = \begin{pmatrix} (y, v_1) \\ \vdots \\ (y, v_n) \end{pmatrix}$$

and let $K_n = r_n K$ and $y_n = r_n y$. Then a finite dimensional version of (2) may be written as

$$K_n x_n = y_n \tag{6}$$

where $x_n = K_n^\dagger y_n$ and the finite dimensional versions of the regularized approximations (4) and (5) are

$$x_{\alpha,n} = U_\alpha(K_n^* K_n) K_n^* y_n \text{ and } x_{\alpha,n}^\delta = U_\alpha(K_n^* K_n) K_n^* y_n^\delta \tag{7}$$

where $y_n^\delta = r_n y^\delta$. We assume that $\delta = \delta(n)$ is such that $\|y_n - y_n^\delta\|_{\mathbb{R}^n} \le \delta$. Note that for the interpretation of this information in the infinite dimensional context, also the basis functions v_i play a role: If $y, y^{\delta'} \in H_2$ are such that $\|P_n y - P_n y^{\delta'}\| \le \delta'$ and if $y_n := r_n y$, $y_n^{\delta'} := r_n y^{\delta'} \in \mathbb{R}^n$ (where P_n denotes the orthogonal projector onto span $\{v_1, \ldots, v_n\}$), then $\|P_n y - P_n y^{\delta'}\|_{H_2}^2 = (y_n - y_n^{\delta'})^T R_n (y_n - y_n^{\delta'})$, where R_n is the matrix with entries (v_i, v_j). Thus, if the $\{v_i\}$ are an orthonormal basis, the error in $P_n y$ in the norm of H_2 is the same as the error in y_n in the norm of $\mathbb{R}^n$. However, if the basis is not orthogonal, an error of δ in y_n can result in a larger error in $P_n y$, since $\|P_n y - P_n y^{\delta'}\|_{H_2}^2 \le \bar{\lambda}_n \cdot \|y_n - y_n^{\delta'}\|_{\mathbb{R}^n}^2$, where $\bar{\lambda}_n$ is the largest eigenvalue of R_n. For this point, cf. also [4, Remark 11].

Note that the adjoint $K_n^*: \mathbb{R}^n \to H_1$ of the operator K_n is given by

$$K_n^* \underset{\sim}{z} = \sum_{i=1}^n z_i K^* v_i \ .$$

It is known that $\|x_n - K^\dagger y\| \to 0$ as $n \to \infty$ (see [4], [8]). We now derive a condition for the convergence of $\|x_n - x_{\alpha,n}\|$ to zero as $n \to \infty$.

The condition depends upon the quantity

$$\omega(\alpha,n) = \max\{|1 - \lambda U_\alpha(\lambda)| : \lambda \in \sigma(K_n^* K_n)\} \tag{8}$$

where $\sigma(K_n^* K_n)$ is the spectrum of the operator $K_n^* K_n$.
Note that $K_n^* K_n$ is a finite rank operator given by

$$K_n^* K_n u = \sum_{i=1}^{n} (Ku, v_i) K^* v_i .$$

Since $R(K_n^* K_n) \subseteq \text{span}\{K^* v_1, \ldots K^* v_n\}$, it follows that $K_n^* K_n u = \lambda u$ if and only if

$$(K_n^* K_n u, K^* v_j) = \lambda (u, K^* v_j) \quad \text{for } j = 1, \ldots, n,$$

or equivalently

$$\sum_{i=1}^{n} (Ku, v_i)(K^* v_i, K^* v_j) = \lambda (Ku, v_j), \quad j = 1, \ldots, n \ .$$

That is, $K_n^* K_n u = \lambda u$ if and only if

$$Q_n K_n u = \lambda K_n u$$

where Q_n is the self-adjoint matrix with entries $(K^* v_i, K^* v_j)$. Therefore the spectrum, $\sigma(K_n^* K_n)$, of $K_n^* K_n$ consists of the eigenvalues of Q_n. Thus,

$$\omega(\alpha,n) = \max\{|1 - \lambda U_\alpha(\lambda)| : \lambda \in \sigma(Q_n)\}. \tag{9}$$

We now show that if the parameter α is related to n in an appropriate fashion then the approximations $x_{\alpha,n}$ converge to $K^\dagger y$ as $n \to \infty$.

Proposition 1. If $\alpha = \alpha(n) \to 0$ as $n \to \infty$ in such a way that $\omega(\alpha,n) \to 0$, where ω is defined by (9), then $\|x_n - x_{\alpha,n}\| \to 0$ as $n \to \infty$.

Proof: Since $y_n = K_n x_n$ and $U_\alpha(K_n^* K_n) K_n^* K_n = K_n^* K_n U_\alpha(K_n^* K_n)$, we have by (7) and the functional calculus of self-adjoint operators that

$$\begin{aligned} \|x_n - x_{\alpha,n}\| &= \| x_n - U_\alpha(K_n^* K_n) K_n^* y_n \| \\ &= \|(I - K_n^* K_n U_\alpha(K_n^* K_n)) x_n\| \\ &\leq \omega(\alpha,n) \ \|x_n\|; \end{aligned}$$

thus, the result follows since (as mentioned above) $\|x_n - K^\dagger y\| \to 0$ and hence $\|x_n\|$ is bounded. □

The perturbation error arising from inexact data can be controlled in a similar way by choosing the regularization parameter as a function of n and δ. The choice depends upon the quantity

$$g(\alpha,n) = \max\{|U_\alpha(\lambda)| : \lambda \in \sigma(K_n K_n^*)\}. \tag{10}$$

Note that the operator $K_n K_n^*$ is represented by the matrix Q_n in the usual coordinate system for $\mathbb{R}^n$ since

$$(K_n K_n^* \underset{\sim}{y})_i = (K(\sum_{j=1}^n y_j K^* v_j),\ v_i)$$

$$= \sum_{j=1}^n (K^* v_i, K^* v_j) y_j = (Q_n \underset{\sim}{y})_i.$$

Hence $\sigma(K_n K_n^*)$ also consists of the eigenvalues of Q_n, so that

$$g(\alpha,n) = \max\{|U_\alpha(\lambda)| : \lambda \in \sigma(Q_n)\}. \tag{11}$$

Proposition 2. If $\alpha = \alpha(n) \to 0$ and $\delta = \delta(n) \to 0$ as $n \to \infty$ in such a way that $\delta\sqrt{g(\alpha,n)} \to 0$, where $g(\alpha,n)$ is defined by (11), then $\|x_{\alpha,n} - x_{\alpha,n}^\delta\| \to 0$ as $n \to \infty$.

Proof: Note that by (7) and the functional calculus of self-adjoint operators,

$$\|x_{\alpha,n} - x_{\alpha,n}^\delta\|^2 = (U_\alpha(K_n^* K_n) K_n^*(y_n - y_n^\delta), U_\alpha(K_n^* K_n) K_n^*(y_n - y_n^\delta))$$

$$= (K_n K_n^* U_\alpha(K_n K_n^*)(y_n - y_n^\delta), U_\alpha(K_n K_n^*)(y_n - y_n^\delta))$$

$$\le C\delta^2 g(\alpha,n)$$

where C is a constant. □

It follows from the proof that as in the infinite dimensional situation mentioned in the introduction, $\sqrt{g(\alpha,n)}$ could be replaced by $h(\alpha,n) := \sup\{\lambda U_\alpha(\lambda)^2 : \lambda \in \sigma(Q_n)\}^{1/2}$.

In most cases of interest the functions $|U_\alpha(\lambda)|$ and $|1 - \lambda U_\alpha(\lambda)|$ are decreasing functions of λ for each $\alpha > 0$. It then follows that (if also $|\lambda U_\alpha(\lambda)| \leq 1$) under the assumptions of Proposition 1,

$$\delta^2 g(\alpha,n) = \delta^2 U_\alpha(\lambda_n) = \frac{\delta^2}{\lambda_n}(1 - (1 - \lambda_n U_\alpha(\lambda_n)))$$

$$= \frac{\delta^2}{\lambda_n}(1 - \omega(\alpha,n)) = \frac{\delta^2}{\lambda_n}(1 - o(1))$$

where λ_n is the smallest eigenvalue of Q_n. Therefore in such cases the condition $\delta\sqrt{g(\alpha,n)} \to 0$ as $n \to \infty$ is equivalent to $\delta = o(\lambda_n^{1/2})$ as $n \to \infty$, which is a condition that is necessary and sufficient also for certain methods of regularization by projection (cf. [4, Theorem 9]). The results above, taken together, give sufficient conditions for the convergence of general projection-regularization methods. In the next section we illustrate these conditions for some specific methods.

3. Some Examples

In the examples presented here , $U_\alpha(\lambda)$ and $1 - \lambda U_\alpha(\lambda)$ (≥ 0) are decreasing as functions of λ and hence each of the conditions $\omega(\alpha,n) \to 0$ and $\delta\sqrt{g(\alpha,n)} \to 0$ can be interpretted in terms of the smallest eigenvalue λ_n of the matrix Q_n as outlined at the end of Section 2. In essence the conditions say that λ_n may not go to zero too rapidly (i.e., n may not be increased too quickly) relative to α and δ.

Consider first the case of Tikhonov regularization, that is, $U_\alpha(\lambda) = (\lambda+\alpha)^{-1}$. In this case

$$\omega(\alpha,n) = \max\{\frac{\alpha}{\lambda+\alpha} : \lambda \in \sigma(K_n^* K_n)\} = \frac{\alpha}{\lambda_n+\alpha} .$$

Hence a sufficient condition for convergence is

$\alpha = o(\lambda_n)$ and $\delta = o(\lambda_n^{1/2})$.

In the case of Tikhonov regularization, it is especially easy to illustrate the difference between regularization-projection and projection-regularization methods:

First, consider the projection-regularization method defined by (7) with $U_\alpha(\lambda) = (\lambda + \alpha)^{-1}$, i.e., for $\alpha > 0$,

$$(\alpha I + K_n^* K_n) x_{\alpha,n} = K_n^* y_n. \tag{12}$$

Using the representation of K_n^* given in Section 2 and the fact (following from (12)) that $x_{\alpha,n} \in \text{span}\{K^*v_1,\ldots,K^*v_n\}$, we can write

$$x_{\alpha,n} = \sum_{i=1}^{n} \bar{\beta}_i K^* v_i \tag{13}$$

where $\bar{\beta} = (\bar{\beta}_1,\ldots,\bar{\beta}_n)$ is defined by the linear system

$$(\alpha I + Q_n)\bar{\beta} = y_n. \tag{14}$$

Since Q_n is regular, we can define $z_n := Q_n^{-1/2} y_n$. With this definition, we obtain from (14) that $\bar{\beta}$ minimizes the functional

$$\beta \to \|Q_n^{1/2}\beta - z_n\|^2_{\mathbb{R}^n} + \alpha \|\beta\|^2_{\mathbb{R}^n} \tag{15}$$

over $\mathbb{R}^n$, while $x_{\alpha,n}$ minimizes the functional

$$x \to \|K_n x - y_n\|^2_{\mathbb{R}^n} + \alpha\|x\|^2 \tag{16}$$

over H_1.

A regularization-projection method would be defined as follows (cf. [8,p.73], [5]): Let $\{u_1,u_2,\ldots\}$ be linearly independent vectors in H_1 (w.l.o.g. in $N(K)^\perp$) such that $\bigcup_{n=1}^{\infty} \text{span}\{u_1,\ldots,u_n\}$ is dense in H_1. Let $\hat{x}_{\alpha,n}$ be determined by

$$(\alpha I + \hat{K}_n^* \hat{K}_n)\hat{x}_{\alpha,n} = \hat{K}_n^* y, \tag{17}$$

where $\hat{K}_n := K_n|_{\text{span}\{u_1,\ldots,u_n\}}$. Then

$$\hat{x}_{\alpha,n} = \sum_{i=1}^{n} \bar{\lambda}_i u_i, \tag{18}$$

where $\bar{\lambda} = (\bar{\lambda}_1,\ldots,\bar{\lambda}_n)$ is defined by the linear system

$$(\alpha M_n + B_n)\,\bar{\lambda} = w_n \tag{19}$$

where M_n and B_n are the matrices with entries (u_i,u_j) and (Ku_i,Ku_j), respectively, and $w_n = ((Ku_1,y),\ldots,(Ku_n,y))^T$. Again, one can characterize $\bar{\lambda}$ and $\hat{x}_{\alpha,n}$ in a variational way: $\bar{\lambda}$ minimizes the functional

$$\lambda \to \|B_n^{1/2}\lambda - r_n\|^2_{\mathbb{R}^n} + \alpha\|M_n^{1/2}\lambda\|^2 \tag{20}$$

(with $r_n := B_n^{-1/2}w_n$) over $\mathbb{R}^n$, while $\hat{x}_{\alpha,n}$ minimizes the functional

$$x \to \|Kx - y\|^2 + \alpha\|x\|^2 \tag{21}$$

over $\operatorname{span}\{u_1,\ldots,u_n\}$.

A comparison between (16) and (21) and (15) and (20) shows the difference between the two methods. If we choose $u_i := K^* v_i$, we can directly compare these methods. (In this case, $M_n = Q_n$.) We carry out this comparison for two different choices of basis functions:

First, let K be compact with singular system $(\sigma_n;\varphi_n,\psi_n)$ and let $v_i := \psi_i$, $u_i := K^*\psi_i = \sigma_i\varphi_i$. Then $Q_n = M_n$ is diagonal with entries $\sigma_1^2,\ldots,\sigma_n^2$, $B_n = Q_n^2$. Thus, the functional in (14) has the form $\beta \to \sum_{i=1}^{n} ((\sigma_i\beta_i - \sigma_i^{-1}y_n^i)^2 + \alpha\beta_i^2)$, while the functional in (20) has the form $\lambda \to \sum_{i=1}^{n} (\sigma_i^2\lambda_i - y_n^i)^2 + \alpha\sigma_i^2\lambda_i^2)$.

Although these functionals are different, their minimizers coincide: $\lambda_i = \beta_i = \dfrac{y_n^i}{\alpha + \sigma_i^2}$. Thus, in this case, both methods coincide and $x_{\alpha,n} = \hat{x}_{\alpha,n} = \sum_{i=1}^{i_n} \dfrac{\sigma_i}{\alpha+\sigma_i^2}(y,\psi_i)\varphi_i$, which can be interpretted as a regularized and truncated singular value expansion.

The other case we want to study is the case that K is induced by an integral operator like in (1) with a continuous kernel k and that the v_i are defined as point evaluation functionals as follows (cf. [15],[2],[3]).

Let Q be the reproducing kernel for the RKHS $H_Q := \overline{R(K)}$, i.e., $Q(s,t) := \int_a^b k(s,\tau)k(t,\tau)d\tau$ and let $s_1, s_2, \ldots$ be distinct points in [a,b] such that $\lim_{n\to\infty} \sup\{\inf\{|s - s_i| : 1 \le i \le n\} : s \in [a,b]\} = 0$ holds.

Let $v_i := Q_{s_i} := Q(s_i,.) \in H_Q =: H_2$. The inner product in H_Q will be denote by $(\ ,\ )_Q$. Then for any $f \in H_Q$, $(f,v_i)_Q = f(s_i)$. If we denote by K^* the adjoint of $K: H_1 \to H_Q$, we have that for any $z \in H_Q$, $w \in H_1$, $(K^*z,w) = (z,Kw)_Q = (K^\dagger z, K^\dagger Kw) = (K^\dagger z, w)$, so that $K^* = K^\dagger$. Hence, $u_i = K^* v_i = K^\dagger Q_{s_i} = k_{s_i} := k(s_i,.)$, $Ku_i = v_i$. Hence, $B_n = M_n = Q_n$ all have the entries $Q(s_i,s_j)$. Thus, (14) becomes

$$(\alpha I + Q_n)\vec{\beta} = (y(s_1),\ldots,y(s_n))^T, \tag{22}$$

while (19) becomes

$$(1+\alpha)Q_n\vec{\lambda} = (y(s_1),\ldots,y(s_n))^T. \tag{23}$$

A comparison of (22) and (23) shows that the projection-regularization method (leading to (22)) and the regularization-projection method (leading to (23)) are different here: The latter method is nothing but least-squares collocation with the right-hand side divided by $(1 + \alpha)$ (cf. [2]).

Of course also iterated Tikhonov regularization (cf. [11]) fits into the framework of the setting developed in Section 2, as do iterative methods. In this case the regularization parameter is a positive integer $m = [\frac{1}{\alpha}]$ which represents an iteration number. The simplest iterative

method is Landweber-Fridman iteration (see [7],[11])

$$x_m = (I - K^*K)x_{m-1} + K^*y, \qquad x_o = 0$$

(we assume here that equation (2) has been scaled so that $\|K\| < 1$).

This can be expressed as

$$x_m = U_m(K^*K)K^*y$$

where

$$U_m(\lambda) = \frac{1 - (1 - \lambda)^m}{\lambda} .$$

In this case $\omega(m,n) = (1 - \lambda_n)^m$ and hence a sufficient condition for convergence of the induced projection-regularization method is that $m \to \infty$ as $n \to \infty$ in such a way that $(1 - \lambda_n)^m \to 0$ and $\delta = o(\lambda_m^{1/2})$.

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