NEW RESULTS ON THE EQUIVALENCE OF REGULARIZATION AND TRUNCATED ITERATION FOR Ill-POSED PROBLEMS

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Setembro RP 30/92

Relatório de Pesquisa

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ABSTRACT - We prove that solutions by direct regularization of linear systems are equivalent to truncated iterations of certain type of iterative methods. Our proofs extend previous results of H. Fleming to the rank-deficient case. We give a unified approach that includes the undetermined and overdetermined problems.

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Setembro - 1992

This work is part of the author's PhD dissertation advised by Dr. A.R. De Pierro.

New Results on the Equivalence of Regularization and Truncated Iteration for Ill-posed Problems

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Abstract

We prove that solutions by direct regularization of linear systems are equivalent to truncated iterations of certain type of iterative methods. Our proofs extend previous results of H. Fleming to the rank-deficient case. We give a unified approach that includes the undetermined and overdetermined problems.

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This research was partially supported by CAPES-PICD.

1. Introduction

Many inverse problems begin with a mathematical model that is a linear Fredholm integral equation of the first kind. After discretization, the problem reduces to solve a system of linear algebraic equations of the form

$$Ax = b\,, \tag{1}$$

where A is a real $m \times n$ matrix, b the m-vector of observations and x an n-vector to be determined. Unfortunately (1) is usually very ill-posed and small perturbations in b generate large errors in the solution, even if we consider minimum-norm solutions in the least squares sense. The standard way to obtain stable solutions is to modify the problem substituting (1) by the Tikhonov regularization [1]. That is the solution is obtained by minimizing the functional

$$F_\alpha(x) = ||Ax - b||^2 + \alpha||L(x - x^0)||^2\,, \tag{2}$$

where the second term in (2) represents some "a priori" information about the problem. L is usually a derivative operator imposing some smoothing constraints on the solution, α a positive regularization parameter controlling the amount of smoothing and x^0 an estimate of x. $||\cdot||$ denotes the square norm in $\mathbb{R}^n$.

Another way to solve (1) is to apply an iterative method to the normal equations

$$A^tAx = A^tb\,. \tag{3}$$

A tipical algorithm for solving (3) is the generalized Landweber-Fridman iteration [2] given by

$$x^{k+1} = x^k + DA^t(b - Ax^k)\,, \qquad k = 0, 1, 2, \ldots \tag{4}$$

where $D = F(A^tA)$ and F is a polynomial or rational function with the property $0 < \lambda F(\lambda) < 2$ for $0 < \lambda < 1$. At the beginning of the process, the accuracy of the iterates improves, but after some time a deteriorating effect shows up due to ill-conditioning. A stable solution can be found by using an appropriate stopping rule that chooses an iterate x^k before this effect comes up. This procedure, known as truncated iteration, establishes a balance between accuracy (to what extend (1) is satisfied) and smoothing requirements similar to those represented by the first and second terms in (2) respectively.

Recently [3], H. Fleming established an equivalence between the two types of methods if A is a full rank matrix. In [3] is proven that every direct regularization method of a very general type for the solution of (1) is equivalent to a truncated iterative method and viceversa. This is done considering separately the overdetermined (rank $A = n < m$) and the underdetermined (rank $A = n > m$) cases. In this paper we extend these results to incomplete rank matrices. Our approach uses a specially derived formula for general iterative methods that allows a simpler and unified proof. Moreover, our proof is valid for methods more general than (4).

In the next section we give some preliminary results for general linear iterative methods that include the formula just mentioned. Section 3 contains our main equivalence results.

2. Preliminary Results

We consider now iterative methods of the form

$$x^{k+1} = Gx^k + f \,, \tag{5}$$

where G is an $n \times n$ matrix and f is a vector in $I\!R^n$. It is clear that if $\{x^k\}$ converges to x^*, this limit point solves the system

$$(I - G)x = f \,. \tag{6}$$

Recall that a matrix G is said to be convergent if $\lim_{k \to \infty} G^k$ exists and this limit exists if and only if the following conditions are verified (see [4]):

(a) The spectral radius of G is less or equal to one.

(b) If λ is an eigenvalue of G such that $|\lambda| = 1$, then $\lambda = 1$ and all the elementary divisors that correspond to λ are linear, i.e., λ has no principal vectors.

The next Theorem describes the iterates generated by (5).

Theorem 1. Let G be an $n \times n$ convergent matrix. Then

$$I\!R^n = \mathcal{N}(I-G) \oplus \mathcal{R}(I-G) , \tag{7}$$

where $\mathcal{N}(I-G)$ and $\mathcal{R}(I-G)$ denote the kernel and range of $I-G$ respectively. Moreover, the following expression holds:

$$x^k = x_1^0 + kf_1 + G^k(x_2^0 - (I-G_2)^{-1}f_2) + (I-G_2)^{-1}f_2 , \tag{8}$$

where f_1, $x_1^0 \in \mathcal{N}(I-G)$ and f_2, $x_2 \in \mathcal{R}(I-G)$ are such that $f = f_1 + f_2$, $x^0 = x_1^0 + x_2^0$, and $G_2 = G\Big|_{\mathcal{R}(I-G)}$.

Proof. Using (5), x^k can be written as

$$x^k = G^k x^0 + \sum_{j=0}^{k-1} G^j f . \tag{9}$$

Let W be the subspace generated by the principal vector and eigenvectors associated to the eigenvalues of G different from one. Clearly

$$I\!R^n = \mathcal{N}(I-G) \oplus W . \tag{10}$$

Let $x_1^0, f_1 \in \mathcal{N}(I-G)$ and $x_2, f_2 \in W$ be such that $x^0 = x_1^0 + x_2^0$ and $f = f_1 + f_2$. Defining $\widehat{G}_2 = G\Big|_W$ and applying (9) we obtain that

$$x^k = x_1^0 + kf_1 + \widehat{G}_2^k x_2^0 + \sum_{j=0}^{k-1} \widehat{G}_2^j f_2 . \tag{11}$$

Taking into account that $\widehat{G}_2$ doesn't have one as eigenvalue and that W is $(I-G)$-invariant, then, $I - \widehat{G}_2$ has an inverse and

$$\sum_{j=0}^{k-1} \widehat{G}_2^j = (I - \widehat{G}_2^k)(I - \widehat{G}_2)^{-1} . \tag{12}$$

Therefore, using (11) and (12), we get that

$$x^k = x_1^0 + kf_1 + \widehat{G}_2^k(x_2^0 - (I - \widehat{G}_2)^{-1} f_2) + (I - \widehat{G}_2)^{-1} f_2 \,. \tag{13}$$

It remains to be proved that $W = \mathcal{R}(I - G)$. To do this, we'll use equation (13). If $f \in W$, then $f_1 = 0$ and the sequence $\{x^k\}$ is convergent, therefore (6) is solvable and $f \in \mathcal{R}(I - G)$ (this is a consequence of (13) and the fact that the eigenvalues of $\widehat{G}_2$ are less than one in modulus, but can be deduced also from known results [5]). On the other hand, if $f \in \mathcal{R}(I - G)$ we can take $x^0 = x^*$, a solution of (6). The resulting sequence is convergent because G is a convergent matrix and, by equation (13), f_1 must be zero; so $f \in W$.

We immediately conclude that $\widehat{G}_2 = G_2 = G\Big|_{\mathcal{R}(I-G)}$ and the result follows. ∎

Consider now the regularized problem

$$\text{minimize} \quad ||Ax - b||_P^2 + ||x - a||_Q^2 \,, \tag{14}$$

where $P \in \mathbb{R}^{m\times m}$ and $Q \in \mathbb{R}^{n\times n}$ are symmetric positive matrices, a is a vector in $\mathbb{R}^n$ and the norms are defined by

$$||z||_P^2 = z^t P^{-1} z \tag{15}$$

(the same for Q). Let us also consider a convergent iterative method of the form

$$x^{k+1} = x^k + MA^tP^{-1}(b - Ax^k) \,, \tag{16}$$

where M is a non-singular matrix. Using the notation of the previous section $G = I - MA^tP^{-1}A$.

Lemma 2. The solution x^* of the problem (14) always exists and can be written as

$$x^* = (I + QA^tP^{-1}A)^{-1}(a - d) + d \,, \tag{17}$$

where

$$d = (MA^tP^{-1}A)_2^{-1} MA^tP^{-1}b \quad \text{and} \quad (MA^tP^{-1}A)_2 = MA^tP^{-1}A\Big|_{\mathcal{R}(MA^tP^{-1}A)}$$

Proof. Using standard calculations, it is easy to see that

$$x^* = (I + QA^tP^{-1}A)^{-1}(QA^tPb + a)\,. \tag{18}$$

By Theorem 1, $(MA^tP^{-1}A)_2$ has an inverse and by adding and substracting $(I + QA^tP^{-1}A)^{-1}(MA^tP^{-1}A)_2^{-1}\,MA^tP^{-1}b$ in (18) we obtain

$$x^* = (I + QA^tP^{-1}A)^{-1}(a - d) + (I + QA^tP^{-1}A)^{-1}(QA^tP^{-1}b + d)\,. \tag{19}$$

We know that the system

$$A^tP^{-1}b = A^tP^{-1}Ax \tag{20}$$

has a solution; so, applying M in both sides of (20) we deduce that $MA^tP^{-1}b \in \mathcal{R}(MA^tP^{-1}A)$ and using this fact we get that

$$MA^tP^{-1}b = MA^tP^{-1}Ad \tag{21}$$

Substituting M by Q in (21) (we can do it because they are nonsingular), (21) implies that

$$QA^tP^{-1}b = (QA^tP^{-1}A)(MA^tP^{-1}A)_2^{-1}MA^tP^{-1}b\,. \tag{22}$$

From (22) we get that

$$(I + QA^tP^{-1}A)^{-1}(QA^tP^{-1}b + d) = d\,. \tag{23}$$

Substituting in (19), the result follows.

∎

3. Equivalence of solutions.

We present in this section the main equivalence results of this paper.

Theorem 3. Every regularized solution of the system (1) has an equivalent truncated iterative solution of the form (16); i.e., given the matrices P and Q in (14) and a positive ıteger k_0 there exists a matrix M such that x^{k_0} given by (16) solves (14).

'roof. Being Q and $A^tP^{-1}A$ symmetric and Q^{-1} positive definite, we can simultaneously iagonalize them; i.e., there exists a nonsingular matrix X such that

$$X^tQ^{-1}X = \mathrm{diag}(\frac{1}{q_1}, \ldots, \frac{1}{q_n}) \tag{24}$$

nd

$$X^tA^tP^{-1}AX = \mathrm{diag}(p_1, \ldots, p_n)\,, \tag{25}$$

ʼith $q_i > 0$ and $p_i \geq 0$ for $i = 1, \ldots, n$. (See [6], section 8.6). Consequently

$$X^{-1}QA^tP^{-1}AX = X^{-1}QX^{-t}(X^tA^tP^{-1}AX) = \mathrm{diag}(p_1q_1, \ldots, p_nq_n)\,. \tag{26}$$

Given a truncation index k_0, let

$$M = X\ \mathrm{diag}(\lambda_1, \ldots, \lambda_n)X^t = XDX^t \tag{27}$$

vhere

$$\lambda_i = \begin{cases} \frac{1}{p_i}[1-(1+p_iq_i)^{-1/k_0}]\,, & \text{if} \quad p_i \neq 0\,, \\ \\ 0\,, & \text{otherwise.} \end{cases} \tag{28}$$

Jsing (26), (27) and (28) we get that

$$\begin{aligned} (I - MA^tP^{-1}A)^{k_0} &= (I - XDX^tA^tP^{-1}A)^{k_0} = \{X(I - DX^tA^tP^{-1}AX)X^{-1}\}^{k_0} \\ &= \{X\ \mathrm{diag}(1-\lambda_ip_i)X^{-1}\}^{k_0} = \\ &= X\mathrm{diag}(1-\lambda_ip_i)^{k_0}X^{-1} = \\ &= X\ \mathrm{diag}(1+p_iq_i)^{-1}X^{-1} = \\ &= (I + QA^tP^{-1}A)^{-1}. \end{aligned} \tag{29}$$

Now

$$I - MA^tP^{-1}A = X\ \mathrm{diag}(1 + p_iq_i)^{-1/k_0} X^{-1}\ ;$$

therefore, M given by (27) defines a method (16) that is convergent.

It remains to be proved that $x^{k_0} = x^*$ the solution of problem (14). By Lemma 2 the expression (17) is valid. If we set $x^0 = a$ and we apply (29), it follows that

$$x^* = (I + QA^tP^{-1}A)^{-1}x_1^0 + (I - MA^tP^{-1}A)^k(x_2^0 - d) + d\ , \tag{30}$$

where $x_1^0 \in \mathcal{N}(MA^tP^{-1}A)$ and $x_2^0 \in \mathcal{R}(MA^tP^{-1}A)$ are such that $x^0 = x_1^0 + x_2^0$. But

$$(I + QA^tP^{-1}A)^{-1}x_1^0 = x_1^0\ , \tag{31}$$

because $x_1^0 \in \mathcal{N}(MA^tP^{-1}A) = \mathcal{N}(A)$. Thus, by Theorem 1, $x^* = x^k$. ∎

We now state and prove the converse of Theorem 3.

Theorem 4. Every truncated-iterative solution of the form (16), where M is a symmetric positive definite matrix, is the solution of a regularized problem of the form (14); i.e., for every k and matrices M and P, there exists a matrix Q such that x^k in (16) solves (14).

Proof. Being M^{-1} and $A^tP^{-1}A$ symmetric and M^{-1} positive definite, we can simultaneoulsy diagonalize them; i.e., there exists a nonsingular matrix Y such that

$$Y^tM^{-1}Y = \mathrm{diag}(1/_{m_1,\ldots,}1/_{m_n})\ ,\ , \tag{32}$$

and

$$Y^t(A^tP^{-1}A)Y = \mathrm{diag}(a_1, \ldots, a_n)\ , \tag{33}$$

with $a_i \geq 0$ and $m_i > 0$ for $i = 1, \ldots, n$.

Define

$$Q = Y\,\mathrm{diag}(\mu_i)Y^t\ , \tag{34}$$

where

$$\mu_i = \begin{cases} \frac{1}{a_i}[(1 - a_im_i)^{-k} - 1]\ , & \text{if} \quad a_i \neq 0\ , \\ 1\ , & \text{otherwise.} \end{cases} \tag{35}$$

Using (32), (33), (34) and (35) we get that

$$
\begin{aligned}
(I + QA^tP^{-1}A)^{-1} &= Y\,\mathrm{diag}(1+\mu_i a_i)^{-1}Y^{-1} \\
&= Y\,\mathrm{diag}(1-a_i m_i)^k Y^{-1} = \\
&= (I - MA^tP^{-1}A)^k . \qquad (36)
\end{aligned}
$$

The method (16) is convergent, then, it must be $1 - a_i m_i < 1$, if $a_i \neq 0$, for $i = 1, \ldots, n$, implying that $\mu_i > 0$. Hence, Q is positive definite. We can apply Theorem 1 and (36) to obtain

$$x^k = x_1^0 + (I + QA^tP^{-1}A)^{-1}(x_2^0 - d) + d\,, \qquad (37)$$

But $x_1^0 \in \mathcal{N}(A)$, then

$$x_1^0 = (I + QA^tP^{-1}A)^{-1}x_1^0\,. \qquad (38)$$

If we set $a = x^0$, and using Lemma 2, $x^k = x^*$.

■

Acknowledgement. I would like to thank Prof. Alvaro R. De Pierro for supervising this work, that is part of my Doctoral Dissertation.

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