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Equivalence of Regularization and Truncated Iteration for General 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. E. Fleming to the rank-deficient case. We give a unified approach that includes the undetermined and overdetermined problems.

1. INTRODUCTION

Many inverse problems begin with a Fredholm integral equation of the first kind. After discretization, the problem reduces to solving a system of linear-algebraic equations of the form

$$Ax = b, \tag{1.1}$$

where A is a real $m \times n$ matrix, b is the m-vector of observations, and x is an n-vector to be determined. Unfortunately (1.1) is usually very ill posed, and small perturbations in b generate large errors in x, even if we consider minimum-norm solutions in the least-squares sense. The standard way to obtain stable solutions is to modify the problem, replacing (1.1) with the Tikhonov regularization [1, 6, 10]. That is, the solution is obtained by

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minimizing the functional

$$F_\alpha(x) = ||Ax - b||^2 + \alpha||L(x - x^0)||^2. \tag{1.2}$$

The second term in (1.2) represents some *a priori* information about the problem. L is usually a derivative operator imposing some smoothing constraints on the solution, α is a positive regularization parameter controlling the amount of smoothing, and x^0 is an estimate of x. Here, $||\cdot||$ denotes the square norm in $\mathbb{R}^n$.

Another way to solve (1.1) is to apply an iterative method to the normal equations

$$A^tAx = A^tb. \tag{1.3}$$

A typical algorithm for solving (1.3) is the generalized Landweber-Fridman iteration [8, 9], which is given by

$$x^{k+1} = x^k + DA^t(b - Ax^k), \qquad k = 0, 1, 2, \ldots, \tag{1.4}$$

where $D = F(A^tA)$ and F is a polynomial or rational function. 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 using a stopping rule to choose an iterate x^k before this effect shows up. This procedure, known as truncated iteration, establishes a balance between accuracy and smoothing requirements similar to those represented by the first and second terms in (1.2).

Recently [4], Fleming established an equivalence between the two types of methods if A has full rank. In [4], it is proven that every direct regularization method of a very general type for the solution of (1.1) is equivalent to a truncated iterative method and vice versa. This is done by considering separately the overdetermined ($n < m$) and the underdetermined ($n > m$) cases. In this paper we extend these results to incomplete-rank matrices. We use a formula for general iterative methods that allows a simpler and unified proof. Moreover, our proof is valid for methods more general than (1.4).

It is known that both methods, Tikhonov regularization and truncated iteration, belong to the class of *spectral approximation schemes*, that is, the regularized approximations can be expanded using the same eigenfunction set, differing only in the choice of the so-called *filter functions* (see, e.g., [6, 7, 11]). In this paper and Fleming's [4], it is shown that the latter form is also a particular case of the former.

In the next section we give 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 iterative methods of the form

$$x^{k+1} = Gx^k + f, \tag{2.1}$$

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

$$(I - G)x = f. \tag{2.2}$$

A matrix G is said to be convergent if $\lim_{k\to\infty} G^k$ exists. This limit exists if and only if the following conditions are verified (see [12]):

(a) The spectral radius of G is less than 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 range and the null space of a matrix A will be denoted by $\mathcal{R}(A)$ and $\mathcal{N}(A)$, respectively. If G is a convergent matrix, then $\mathrm{ind}(I-G) \le 1$, where $\mathrm{ind}(A)$ stands for the index of A (i.e., the smallest nonnegative integer q such that $\mathcal{R}(A^q) = \mathcal{R}(A^{q+1})$ holds; cf. [2, Definition 7.2.1]). If $\mathrm{ind}(A) = q$, then $\mathbb{R}^n = \mathcal{N}(A^q) \oplus \mathcal{R}(A^q)$ (cf. [2, Lemma 7.2.1]). Thus, if G is a convergent matrix, then $\mathbb{R}^n = \mathcal{N}(I - G) \oplus \mathcal{R}(I - G)$.

The following theorem describes the iterates generated by (2.1).

THEOREM 2.1. *Let G be an $n \times n$ convergent matrix. Then*

$$\mathbb{R}^n = \mathcal{N}(I - G) \oplus \mathcal{R}(I - G), \tag{2.3}$$

and the following expression holds:

$$x^k = x_1^0 + kf_1 + G^k\left[x_2^0 - (I - G_2)^{-1}f_2\right] + (I - G_2)^{-1}f_2, \tag{2.4}$$

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 $G_2 = G|_{\mathcal{R}(I-G)}$.

Proof. Using (2.1), x^k can be written as

$$x^k = G^k x^0 + \sum_{j=0}^{k-1} G^j f. \tag{2.5}$$

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

$$\mathbb{R}^n = \mathcal{N}(I-G) \oplus W. \tag{2.6}$$

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 $\widehat{G}_2 = G|_W$ and applying (2.5), we obtain

$$x^k = x_1^0 + kf_1 + \widehat{G}_2^k x_2^0 + \sum_{j=0}^{k-1} \widehat{G}_2^j f_2. \tag{2.7}$$

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

$$\sum_{j=0}^{k-1} \widehat{G}_2^j = (I-\widehat{G}_2^k)(I-\widehat{G}_2)^{-1}. \tag{2.8}$$

Therefore, using (2.7) and (2.8), we get that

$$x^k = x_1^0 + kf_1 + \widehat{G}_2^k\left[x_2^0 - (I-\widehat{G}_2)^{-1} f_2\right] + (I-\widehat{G}_2)^{-1} f_2. \tag{2.9}$$

It remains to be proved that $W = \mathcal{R}(I-G)$. To do this, we will use Equation (2.9). If $f \in W$, then $f_1 = 0$ and the sequence $\{x^k\}$ is convergent; therefore (2.2) is solvable and $f \in \mathcal{R}(I-G)$ (this is a consequence of (2.9) and the fact that the eigenvalues of $\widehat{G}_2$ are less than one in modulus, but can be deduced also from [3]). On the other hand, if $f \in \mathcal{R}(I-G)$, then we can take $x^0 = x^*$, a solution of (2.2). The resulting sequence is convergent because G is a convergent matrix and, by Equation (2.9), f_1 must be zero; so $f \in W$.

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

Given the Jordan canonical form of a matrix A,

$$A = P \begin{bmatrix} J_0 & 0 \\ 0 & J_1 \end{bmatrix} P^{-1}$$

(all Jordan blocks belonging to the eigenvalue $\lambda = 0$ of A are collected in J_0), the Drazin inverse A^D of A is

$$A^D = P \begin{bmatrix} 0 & 0 \\ 0 & J_1^{-1} \end{bmatrix} P^{-1}$$

(see e.g. [2, Definitions 7.2.2, 7.2.3 and Theorem 7.2.1]). Thus, the Equation (2.4) can be rewritten as

$$x^k = x_1^0 + kf_1 + G^k\left[x_2^0 - (I-G)^D f\right] + (I-G)^D f.$$

Consider now the regularized problem

$$\text{minimize} \quad ||Ax-b||_P^2 + ||x-a||_Q^2, \tag{2.10}$$

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

$$||z||_P^2 = z^t P^{-1} z \tag{2.11}$$

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

$$x^{k+1} = x^k + MA^tP^{-1}(b - Ax^k), \tag{2.12}$$

where M is a nonsingular matrix. Using the notation of the previous section,

$$G = I - MA^tP^{-1}A.$$

LEMMA 2.2. *The solution x^* of the problem* (2.10) *always exists and can be written as*

$$x^* = (I + QA^tP^{-1}A)^{-1}(a-d) + d, \tag{2.13}$$

where

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

Proof. It is easy to see that

$$x^* = (I + QA^tP^{-1}A)^{-1}(QA^tPb + a). \tag{2.14}$$

By Theorem 2.1, $(MA^tP^{-1}A)_2$ has an inverse, and by adding and subtracting

$$(I + QA^tP^{-1}A)^{-1}(MA^tP^{-1}A)_2^{-1}\,MA^tP^{-1}b$$

in (2.14) we obtain

$$x^* = (I+QA^tP^{-1}A)^{-1}(a-d) + (I+QA^tP^{-1}A)^{-1}(QA^tP^{-1}b+d). \tag{2.15}$$

The system

$$A^tP^{-1}b = A^tP^{-1}Ax \tag{2.16}$$

has a solution. Applying M in both sides of (2.16), we deduce that

$$MA^tP^{-1}b \in \mathcal{R}(MA^tP^{-1}A).$$

Therefore,

$$MA^tP^{-1}b = MA^tP^{-1}Ad \tag{2.17}$$

Since M and Q are nonsingular, we can replace M by Q in (2.17), obtaining

$$QA^tP^{-1}b = (QA^tP^{-1}A)(MA^tP^{-1}A)_2^{-1}MA^tP^{-1}b. \tag{2.18}$$

From (2.18) we get that

$$(I + QA^tP^{-1}A)^{-1}(QA^tP^{-1}b + d) = d. \tag{2.19}$$

The result follows from (2.15). ∎

3. EQUIVALENCE OF SOLUTIONS

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

THEOREM 3.1. *Every regularized solution of the system* (1.1) *has an equivalent truncated iterative solution of the form* (2.12); *i.e., given the matrices P and Q in* (2.10) *and a positive integer k_0, there exists a matrix M such that x^{k_0} given by* (2.12) *solves* (2.10).

Proof. Since Q and $A^tP^{-1}A$ are symmetric and Q^{-1} is positive definite, we can simultaneously diagonalize them. Thus, there exists a nonsingular matrix X such that

$$X^tQ^{-1}X = \text{diag}\left(\frac{1}{q_1}, \dots, \frac{1}{q_n}\right) \tag{3.1}$$

and

$$X^tA^tP^{-1}AX = \text{diag}(p_1, \dots, p_n), \tag{3.2}$$

with $q_i > 0$ and $p_i \geq 0$ for $i = 1, \dots, n$. (See [5, Chapter 8].) Consequently

$$X^{-1}QA^tP^{-1}AX = X^{-1}QX^{-t}(X^tA^tP^{-1}AX) = \text{diag}(p_1q_1, \dots, p_nq_n). \tag{3.3}$$

Given a truncation index k_0, let

$$M = X\,\mathrm{diag}(\lambda_1, \ldots, \lambda_n)\,X^t = XDX^t, \tag{3.4}$$

where

$$\lambda_i = \begin{cases} (1/p_i)[1-(1+p_iq_i)^{-1/k_0}] & \text{if} \quad p_i \neq 0, \\ 1 & \text{otherwise.} \end{cases} \tag{3.5}$$

Using (3.3), (3.4), and (3.5) we get that

$$\begin{aligned}(I - MA^tP^{-1}A)^{k_0} &= (I - XDX^tA^tP^{-1}A)^{k_0} \\ &= \{X(I - DX^tA^tP^{-1}AX)X^{-1}\}^{k_0} \\ &= \{X\,\mathrm{diag}(1-\lambda_ip_i)\,X^{-1}\}^{k_0} \\ &= X\,\mathrm{diag}\,(1-\lambda_ip_i)^{k_0}\,X^{-1} \\ &= X\,\mathrm{diag}(1+p_iq_i)^{-1}\,X^{-1} \\ &= (I + QA^tP^{-1}A)^{-1}. \end{aligned} \tag{3.6}$$

Now

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

therefore, M given by (3.4) defines a method (2.12) that is convergent.

It remains to be proved that $x^{k_0} = x^*$ is the solution of the problem (2.10). By Lemma 2.2, the expression (2.13) is valid. If we set $x^0 = a$ and we apply (3.6), it follows that

$$x^* = (I + QA^tP^{-1}A)^{-1}x_1^0 + (I - MA^tP^{-1}A)^k(x_2^0 - d) + d, \tag{3.7}$$

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

$$(I + QA^tP^{-1}A)^{-1}x_1^0 = x_1^0\,, \tag{3.8}$$

because $x_1^0 \in \mathcal{N}(MA^tP^{-1}A) = \mathcal{N}(A)$. Thus, by Theorem 2.1, $x^* = x^k$. ∎

We now state and prove the converse of Theorem 3.1.

THEOREM 3.2. *Every truncated-iterative solution of the form* (2.12), *where M is a symmetric positive definite matrix, is the solution of a regularized problem of the form* (2.10); *i.e., for every k and matrices M and P, there exists a matrix Q such that x^k in* (2.12) *solves* (2.10).

Proof. Since M^{-1} and $A^tP^{-1}A$ are symmetric and M^{-1} is positive definite, we can diagonalize them simultaneoulsy. Thus, there exists a nonsingular matrix Y such that

$$Y^t M^{-1} Y = \operatorname{diag}\left(\frac{1}{m_1}, \ldots, \frac{1}{m_n}\right), \tag{3.9}$$

and

$$Y^t(A^t P^{-1} A) Y = \operatorname{diag}(a_1, \ldots, a_n), \tag{3.10}$$

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

Define

$$Q = Y \operatorname{diag}(\mu_i) Y^t, \tag{3.11}$$

where

$$\mu_i = \begin{cases} (1/a_i)[(1 - a_i m_i)^{-k} - 1] & \text{if} \quad a_i \neq 0, \\ 1, & \text{otherwise.} \end{cases} \tag{3.12}$$

Using (3.9), (3.10), (3.11), and (3.12), we get that

$$\begin{aligned} (I + QA^t P^{-1} A)^{-1} &= Y \operatorname{diag}(1 + \mu_i a_i)^{-1} Y^{-1} \\ &= Y \operatorname{diag}(1 - a_i m_i)^k Y^{-1} \\ &= (I - MA^t P^{-1} A)^k. \end{aligned} \tag{3.13}$$

The method (2.12) is convergent, so we must have $1 - a_i m_i < 1$, if $a_i \neq 0$, for $i = 1, \ldots, n$, implying that $\mu_i > 0$. Hence, Q is positive definite. We can apply Theorem 2.1 and (3.13) to obtain

$$x^k = x_1^0 + (I + QA^t P^{-1} A)^{-1}(x_2^0 - d) + d, \tag{3.14}$$

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

$$x_1^0 = (I + QA^t P^{-1} A)^{-1} x_1^0. \tag{3.15}$$

If we set $a = x^0$, and using Lemma 2.2, we conclude that $x^k = x^*$. ■

EXAMPLE. Consider the Landweber method [8]

$$x^{k+1} = x^k + \omega A^t(b - Ax^k), \qquad k = 0, 1, 2, \ldots, \tag{3.16}$$

where ω is a positive real number. If O is an orthogonal matrix such that

$$O^t A^t A O = \operatorname{diag}(a_1, \ldots, a_n), \tag{3.17}$$

then, using the proof of Theorem 3.2, x^k is the solution of the problem

$$\text{minimize} \quad ||Ax - b||_2^2 + ||D^{-1/2} O^t x||_2^2, \tag{3.18}$$

where

$$D = \operatorname{diag}(\mu_i) \tag{3.19}$$

and

$$\mu_i = \begin{cases} (1/a_i)[(1-\omega a_i)^{-k} - 1] & \text{if} \quad a_i \neq 0, \\ 1, & \text{otherwise.} \end{cases} \tag{3.20}$$

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