ALGORITHMS FOR THE REGULARIZATION OF ILL-CONDITIONED LEAST SQUARES PROBLEMS

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Abstract.

Two regularization methods for ill-conditioned least squares problems are studied from the point of view of numerical efficiency. The regularization methods are formulated as quadratically constrained least squares problems, and it is shown that if they are transformed into a certain standard form, very efficient algorithms can be used for their solution. New algorithms are given, both for the transformation and for the regularization methods in standard form. A comparison to previous algorithms is made and it is shown that the overall efficiency (in terms of the number of arithmetic operations) of the new algorithms is better.

1. Introduction.

The problem of solving a Fredholm integral equation of the first kind

\[ \int_a^b K(x,y)f(y)dy = g(x), \quad c \leq x \leq d, \quad -\infty < a < b < +\infty, \]

where \( K \) is continuous, is ill-posed in the sense that the solution \( f \) does not depend continuously on the data \( g \). Equation (1.1) can be discretized in various ways, e.g. by moment discretization (see [14]), or expansion of \( f \) in a basis of piece-wise polynomials (see [9]), giving a system of linear equations,

\[ Kf = g, \]

where \( K \) is an \( m \times n \) matrix and \( f \) and \( g \) are vectors.

Due to the ill-posedness of (1.1) the condition number of \( K \) increases rapidly with \( n \). Therefore any attempt to solve (1.2) e.g. in the least squares sense for large values of \( n \) will give a meaningless result, and in this sense the problem of solving (1.2) is ill-posed too. To make it well-posed one can introduce some a priori information about the solution, e.g. in the form of a bound of the norm of \( Lf \), where \( L \) is some \( p \times n \) matrix. This leads to a constrained least squares problem

\[ R1: \min_{f \in B_1} \|Kf - g\|_2, \quad B_1 = \{ f : \|Lf\|_2 \leq \omega \}. \]
In practice $g$ often contains measurement errors and then it is not meaningful to try to satisfy (1.2) exactly. If we know that the solution $f$ is smooth in some sense we are led to the following minimization problem

$$R_2: \min_{f \in B_\varepsilon} \|Lf\|_2, \quad B_\varepsilon = \{f: \|Kf - g\|_2 \leq \varepsilon\},$$

for some value of $\varepsilon$ related to the statistical distribution of the errors in $g$ (see [9] and [1]).

In [3] $R_1$ and $R_2$ are studied and it is proved that in all interesting cases the minima are attained on the boundaries of $B_1$ and $B_2$. Using the terminology of Tihonov [17] we call $R_1$ and $R_2$ regularization methods for the ill-conditioned least squares problem $\min \|Kf - g\|_2$. $R_1$ is sometimes called the method of quasisolution [10]. $R_2$ was suggested by Phillips [15] and Cook [1].

In $R_1$ and $R_2$ the matrix $L$ is the discretization of a differentiation operator and thus in most cases a band matrix. For simplicity we assume that $L$ has full row rank (i.e. $\text{rank}(L) = p$). This is no restriction, since otherwise $L$ can be transformed into a full row rank matrix by premultiplication by an orthogonal matrix [13], Theorem 3.15. We also assume that the nullspaces of $K$ and $L$ intersect trivially:

$$N(K) \cap N(L) = \{0\}. \tag{1.5}$$

This is a necessary condition for (1.3) and (1.4) to have a unique solution.

Using the method of Lagrange multipliers we see that (1.3) and (1.4) are equivalent to solving (for the multiplier $\mu$, $\mu > 0$) the equations

$$h_1(\mu) = \|Lf_\mu\|_2^2 - \omega^2 = 0, \tag{1.6}$$

$$h_2(\mu) = \|Kf_\mu - g\|_2^2 - \varepsilon^2 = 0, \tag{1.7}$$

respectively, where $f_\mu$ is the solution of

$$\min_f \{\|Kf - g\|_2^2 + \mu \|Lf\|_2^2\}. \tag{1.8}$$

Thus we note that the repeated solution of the unconstrained least squares problem (1.8) for different values of $\mu$ is common to $R_1$ and $R_2$. (We also remark that (1.8) in itself has been suggested as a regularization method by Tihonov [17], [18]).

We shall say that $R_1$ and $R_2$ (and also (1.8)) are in standard form if $L = I$.

Although there is an extensive literature about regularization methods, not very much has been written about numerical algorithms for $R_1$ and $R_2$, except when they are in standard form, ([7], [8]). In this paper we develop efficient algorithms for $R_1$ and $R_2$ in the general case $L \neq I$. 