



An iterative algorithm for solving ill-conditioned linear least squares problems

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ABSTRACT

Linear Least Squares (LLS) problems are particularly difficult to solve because they are frequently ill-conditioned, and involve large quantities of data. Ill-conditioned LLS problems are commonly seen in mathematics and geosciences, where regularization algorithms are employed to seek optimal solutions. For many problems, even with the use of regularization algorithms it may be impossible to obtain an accurate solution. Riley and Golub suggested an iterative scheme for solving LLS problems. For the early iteration algorithm, it is difficult to improve the well-conditioned perturbed matrix and accelerate the convergence at the same time. Aiming at this problem, self-adaptive iteration algorithm (SAIA) is proposed in this paper for solving severe ill-conditioned LLS problems. The algorithm is different from other popular algorithms proposed in recent references. It avoids matrix inverse by using Cholesky decomposition, and tunes the perturbation parameter according to the rate of residual error decline in the iterative process. Example shows that the algorithm can greatly reduce iteration times, accelerate the convergence, and also greatly enhance the computation accuracy.

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1. Introduction

A linear or linearized model is expressed as

$$L = AX - V, \quad \text{cov}(V) = \sigma_0^2 Q, \quad P = Q^{-1} \quad (1)$$

where $L \in \mathbb{R}^n$ is an observation vector contaminated by an error vector $V \in \mathbb{R}^n$ with normal distribution of mean zero and

covariance matrix $\sigma_0^2 Q$; P is a positive-definite weight matrix; $A \in \mathbb{R}^{n \times m}$ is a matrix with full column rank connected to an unknown vector $X \in \mathbb{R}^m$ and generally $n > m$. We are concerned with the solution of least-squares problems:

$$\min_{X \in \mathbb{R}^m} \|AX - L\| \quad (2)$$

where $\|\cdot\|$ denotes the Euclidean vector norm, X is the unknown vector to be solved. If the matrix A is well-conditioned,

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the least-squares solution has the best unbiased estimation to this over determined system of equation (1) which is given as

$$\begin{cases} (\mathbf{A}^T \mathbf{P} \mathbf{A}) \mathbf{X} = \mathbf{A}^T \mathbf{P} \mathbf{L} \\ \mathbf{X} = (\mathbf{A}^T \mathbf{P} \mathbf{A})^{-1} (\mathbf{A}^T \mathbf{P} \mathbf{L}) \end{cases} \quad (3)$$

However, $\mathbf{A}^T \mathbf{P} \mathbf{A}$ may be a severely ill-conditioned matrix, thus it cannot be inverted. Problems of this kind are referred to ill-posed problems. Due to the ill-conditioning of $\mathbf{A}^T \mathbf{P} \mathbf{A}$, these problems are difficult to solve accurately [1]. Inverting ill-conditioned large matrices is a challenging problem involved in a wide range of applications, including inverse problems and partial differential equations [2]. Global Navigation Satellite System (GNSS) is a fast, dynamic, high precision positioning technique that has been attracting more and more attention in modern geodesy. In the static positioning of GNSS, the carrier phase ambiguity and other parameters are set as unknown for solving. A linear observational equation system for real-time GNSS carrier phase ambiguity resolution is often severely ill-posed, in the case of poor satellite geometry [3]. Generally, in order to improve the precision and reliability of the solution, a long time for GNSS observing is usually needed. GNSS satellites belong to high orbit satellite, and the angle velocity is small. If the observation period is not long enough, the directions of the receivers to the satellites will see little change, and the distances between stations and satellites vary little in the whole observing session. Thus observation equations of the same satellites and different epochs are almost similar, so to rapidly determine phase ambiguity is a typical ill-condition problem.

Linear discrete ill-posed problems are difficult to solve numerically, because their solution is very sensitive to perturbations which may stem from errors in the data, round-off errors and discretization errors during which introduced the solution process [4,5]. Severely ill-conditioned matrix inverting problems abound in the geosciences, especially in the data processing of modern survey. In the numerical algorithm, all the cases of inappropriate function model or inappropriate calculating method, a morbid or singular iteration matrix and so on, will lead to inaccurate solutions. For singular matrix and ill-posed problems, there are a large number of research results, such as regularization methods. Among all regularization methods, perhaps the best known and most commonly used is the Tikhonov–Phillips method, which was originally proposed by Tikhonov and Phillips in 1962 and 1963 [6]. It's possible that the best understood regularization method is due to Tikhonov [7]. The Tikhonov regularization method is one of the most popular approaches to determine an approximation of \mathbf{X} . This method replaces the linear system of equation (2) by a penalized least-squares problem of the form [8–12]:

$$\min_{\mathbf{X} \in \mathbb{R}^n} \{ \|\mathbf{A}\mathbf{X} - \mathbf{L}\|^2 + \mu \|\mathbf{T}\mathbf{X}\|^2 \} \quad (4)$$

where $\mu > 0$ is known as the regularization parameter, \mathbf{T} is some suitably chosen Tikhonov matrix. Ill-posed problems must be first regularized if one wants to successfully attack the task of numerically approximating their solutions. It is often said that the art of applying regularization methods consist always in maintaining an adequate balance between

accuracy and stability [13]. As to regularization methods, there are three drawbacks: (1) these methods destroy the equivalence relation of the equation (3); (2) a regularized solution is well-known to be biased [14]; and (3) to determine the optimal regularization parameter is rather difficult.

Riley [15] and Golub [16] suggested an iterative scheme for solving LLS problems, which has advantages as follows: (1) it makes the perturbed matrix well-conditioned, and improves the condition number of matrix in the normal equation; (2) it keeps the equivalence relation of the equation unchanged; and (3) the iteration can always converge to the optimal solution theoretically. For these reasons, it has attracted attention from geodesists in data processing widely. However, a few problems are found in its practical application in recent years [17]. The choice of perturbation parameter will greatly affect the rate of convergence of the iterative method, and thus one must choose it with great care [16]. The perturbation parameter chosen should be large enough to make the perturbed matrix well-conditioned, yet small enough to ensure that the error $\|\mathbf{X} - \bar{\mathbf{X}}\|$ is small [18]. If the perturbation parameter increases, the convergence rates turn out to be low; but if decreased, the ill-posed matrix cannot be improved to be well-conditioned. For this reason, based on theoretical analysis and a large number of experiments, a new self-adaptive iteration algorithm is proposed in this paper.

The contributions of this paper are as follows: (1) a formula to determine the initial perturbation parameter is given; (2) a self-adaptive strategy is proposed to determine the tunable perturbation parameter dynamically; (3) an optimal termination point is found to stop the iteration. Comparison results of some experiments indicate that the algorithm can accelerate the convergence and improve computation accuracy. The rest of the paper is organized as follows. Section 2 introduces the algorithm in detail for severe ill-posed problems. Section 3 gives several experiments to demonstrate the superior performance of the proposed algorithm. The concluding remarks are outlined in Section 4.

2. Self-adaptive iteration algorithms

2.1. Implementations of regularization

The ill-posed matrix is generally measured by the condition number of the matrix. If the condition number of $\mathbf{A}^T \mathbf{P} \mathbf{A}$ is very large, that means the matrix is usually ill-posed. In this case, finding the inverse matrix of $\mathbf{A}^T \mathbf{P} \mathbf{A}$ in equation (3) may have no stable solution. To solve the problem, many references [8,18–21] employ an algorithm like this

$$\mathbf{X}_\mu = (\mathbf{A}^T \mathbf{P} \mathbf{A} + \mu \mathbf{I})^{-1} (\mathbf{A}^T \mathbf{P} \mathbf{L}) \quad (5)$$

where μ is an arbitrary regularization parameter, \mathbf{I} denotes identity matrix. It is obvious that adding $\mu \mathbf{I}$ to the right side of equation (5) will destroy the equivalence relation in equation (3). The solution \mathbf{X}_μ solved by equation (5) is no longer the same \mathbf{X} in equation (3). Another drawback is that the condition number of $\mathbf{A}^T \mathbf{P} \mathbf{A}$ is much more than that of \mathbf{A} , which requires μ to be large enough to control the condition of the matrix [18]. Moreover, it is difficulty to determine an

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