



A maximal projection solution of ill-posed linear system in a column subspace, better than the least squares solution



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ABSTRACT

A better method than the least squares solution is proposed in this paper to solve an n -dimensional ill-posed linear equations system $\mathbf{Ax} = \mathbf{b}$ in an m -dimensional column subspace $\mathcal{C}_m$, which is selected in such a way that each column in $\mathcal{C}_m$ is in a closer proximity to $\mathbf{b}$. We maximize the orthogonal projection of $\mathbf{b}$ onto $\mathbf{y} := \mathbf{Ax}$ to find an approximate solution $\mathbf{x} \in \text{span}\{\mathbf{a}, \mathcal{C}_m\}$, where $\mathbf{a}$ is a nonzero free vector. Then, we can prove that the maximal projection solution (MP) is better than the least squares solution (LS) with $\|\mathbf{b} - \mathbf{Ax}_{\text{MP}}\| < \|\mathbf{b} - \mathbf{Ax}_{\text{LS}}\|$. Numerical examples of inverse problems under a large noise maybe up to 30% are discussed which confirm the efficiency of presently developed MP algorithms: MPA and MPA(m).

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1. Introduction

In this paper we are going to derive a proximate column subspace method to find the optimal solution by maximizing the orthogonal projection, instead of that obtained by the method of least squares, to solve the following linear equations system:

$$\mathbf{Ax} = \mathbf{b}, \quad (1)$$

where $\mathbf{x} \in \mathbb{R}^n$ is an unknown vector, and $\mathbf{A} \in \mathbb{R}^{n \times n}$ is a given non-singular and non-symmetric coefficient matrix with $\text{rank}(\mathbf{A}) = n$. The above equation is sometimes obtained via an n -dimensional discretization of a bounded linear operator equation under noisy input. Under this situation, we only look for a generalized solution $\mathbf{x} = \mathbf{A}^\dagger \mathbf{b}$, where $\mathbf{A}^\dagger$ is a pseudo-inverse of $\mathbf{A}$ in the Penrose sense. When $\mathbf{A}$ is severely ill-conditioned and the data $\mathbf{b}$ are corrupted by random noise, we may encounter the problem that the numerical solution of Eq. (1) might deviate from the exact one to a great extent. If we only know the perturbed input data $\mathbf{b}^\delta \in \mathbb{R}^n$ with $\|\mathbf{b} - \mathbf{b}^\delta\| \leq \delta$, and if the problem is ill-posed, i.e., the range($\mathbf{A}$) is not closed or equivalently $\mathbf{A}^\dagger$ is unbounded, we have to solve Eq. (1) by a regularization method.

Given an initial guess $\mathbf{x}_0$, from Eq. (1) we have an initial residual vector:

$$\mathbf{r}_0 = \mathbf{b} - \mathbf{Ax}_0.$$

Upon letting

$$\mathbf{u} = \mathbf{x} - \mathbf{x}_0.$$

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Eq. (1) is equivalent to

$$\mathbf{A}\mathbf{u} = \mathbf{r}_0, \quad (2)$$

which can be used to search a descent direction $\mathbf{u}$ after giving an initial residual vector $\mathbf{r}_0$.

There are several numerical solution methods of Eq. (1), which are originated from the idea of minimization. For the positive definite linear system, solving Eq. (1) by the steepest descent method is equivalent to solving the following minimization problem [1,2]:

$$\min_{\mathbf{x} \in \mathbb{R}^n} \varphi(\mathbf{x}) = \min_{\mathbf{x} \in \mathbb{R}^n} \left[\frac{1}{2} \mathbf{x}^T \mathbf{A} \mathbf{x} - \mathbf{b}^T \mathbf{x} \right]. \quad (3)$$

Liu [3–5] has minimized the following merit function:

$$\min \left\{ a_0 = \frac{\|\mathbf{r}_0\|^2 \|\mathbf{A}\mathbf{u}\|^2}{[\mathbf{r}_0 \cdot (\mathbf{A}\mathbf{u})]^2} \right\}, \quad (4)$$

in order to obtain a fast descent direction $\mathbf{u}$ for a given residual vector $\mathbf{r}_0$ in terms of two or three vectors, used in the iterative solution of Eq. (1). Because the above minimization problem is quite difficult to be solved for finding $\mathbf{u}$ when $\mathbf{u}$ is expressed as a linear combination of multi-vectors, Liu [6] has solved, instead of Eq. (4), a simpler minimization problem in a Krylov subspace:

$$\min \{ \|\mathbf{r}_0 - \mathbf{A}\mathbf{u}\|^2 = \|\mathbf{b} - \mathbf{A}\mathbf{x}\|^2 \}. \quad (5)$$

In the solution of linear equations system the Krylov subspace method is one of the most important classes of numerical methods, and the iterative algorithms applied to solve large-scale linear systems are mostly the preconditioned Krylov subspace methods [6–12]. In the past few decades, the Krylov subspace methods for solving Eq. (1) have been studied in depth since the appearance of pioneering work [13,14], such as the minimum residual algorithm [15], the generalized minimal residual method (GMRES) [9,10], the quasi-minimal residual method [11], the biconjugate gradient method [16], the conjugate gradient squared method [17], and the biconjugate gradient stabilized method [18]. There are more discussions on the Krylov subspace methods in the review papers [8,19] and text books [20,21]. The most studies are paying attention to the residual vector and the “optimality” of some residual errors in the Krylov subspace to derive the “optimal approximation”.

As mentioned by Matinfar et al. [22] some iterative methods like GMRES and LSQR are paying attention to residual vector, and several implementations for the GMRES were assessed for solving ill-posed linear systems. Recently, Liu [23] has developed a new theory to find the double optimal solution of Eq. (1) in a Krylov subspace, by simultaneously basing on the two minimizations in Eqs. (4) and (5). Here, we only use the merit function in Eq. (4) and take advantage of the scaling invariant property of the proposed merit function [24] to derive a *maximal projection solution* (MP) in a proximate column subspace. It would be quite significant that the MP is better than the least squares solution (LS), where an exact equation to measure the difference between the square residuals of MP and LS will be derived.

The remaining parts of this paper are arranged as follows. In Section 2 we start from an m -dimensional column subspace to express the solution with coefficients to be optimized in Section 3, where a new merit function is proposed for finding the optimal expansion coefficients. We can derive a closed-form MP solution of Eq. (1). The comparisons between the MP and the LS are performed in Section 4, and an important improvement is verified. In Section 5 we describe the numerical algorithm based on the MP solution. The examples of linear inverse problems are given in Section 6 to display some advantages of the present methodology to find an approximate solution of Eq. (1). Finally, the conclusions are drawn in Section 7.

2. A proximate column subspace method

Suppose that we have an m -dimensional Krylov subspace, which is generated by the coefficient matrix $\mathbf{A}$ from the right-hand side vector $\mathbf{r}_0$ in Eq. (2):

$$\mathcal{K}_m := \text{span}\{\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \dots, \mathbf{A}^{m-1}\mathbf{r}_0\}. \quad (6)$$

Let $\mathcal{L}_m = \mathbf{A}\mathcal{K}_m$. The idea of GMRES is using the Galerkin method to search the solution $\mathbf{u} \in \mathcal{K}_m$ such that the residual $\mathbf{b} - \mathbf{A}\mathbf{x} = \mathbf{r}_0 - \mathbf{A}\mathbf{u}$ is perpendicular to $\mathcal{L}_m$ [10]. It can be shown that the solution $\mathbf{u} \in \mathcal{K}_m$ minimizes the residual [20].

The idea of projection method, including the GMRES, is searching for a solution $\mathbf{x}$ in a smaller subspace than the original space $\mathbb{R}^n$ with dimension $m \ll n$. In doing so, the higher order expansion terms larger than that in Eq. (6) are truncated, and we can find the lower order expansion coefficients through a suitably designed optimization in a Krylov subspace. A basic ingredient of the Krylov subspace method is the construction of an orthonormal set of linearly independent bases. However, as seen in Eq. (6) the expansion of Krylov matrix consisting of the Krylov vectors is highly ill-conditioned when the coefficient matrix $\mathbf{A}$ is itself a highly ill-conditioned matrix. The more powers of $\mathbf{A}$ in Eq. (6) make the situation of ill-posedness more worse. Instead of the Krylov subspace method, we will construct a column subspace expansion method.

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