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A doubly optimized solution of linear equations system expressed in an affine Krylov subspace

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ABSTRACT

A mathematical procedure for finding a closed-form *double optimal solution* (DOS) of an n-dimensional linear equations system $\mathbf{Bx} = \mathbf{b}$ is developed, which expresses the solution in an m-dimensional affine Krylov subspace with undetermined coefficients, and two optimization techniques are used to determine these coefficients in closed-form. To find the DOS, it is very time saving without the need of any iteration; in practice, we only need to invert an $m \times m$ matrix one time, where $m \ll n$. The DOS is not exactly equal to the exact solution, but it can provide an acceptable approximate solution of linear equations system, whose applicable range is identified. Some properties are analyzed that the DOS is an exact solution of a projected linear system of $\mathbf{Bx} = \mathbf{b}$ onto the affine Krylov subspace. The tests for large scale problems demonstrate the efficiency of DOS on non-sparse linear systems.

1. Introduction

In this paper we derive a closed-form double optimal solution in an affine Krylov subspace for the following linear equations system:

$$\mathbf{Bx} = \mathbf{b}, \tag{1}$$

where $\mathbf{x} \in \mathbb{R}^n$ is an unknown vector, to be determined from a given non-singular coefficient matrix $\mathbf{B} \in \mathbb{R}^{n\times n}$, and the input $\mathbf{b} \in \mathbb{R}^n$. In the text books [1–4] there are many techniques to find the solution of Eq. (1).

Around Eq. (1), there are several solution methods originated from the idea of minimization. For the positive definite linear system, solving Eq. (1) by the steepest descent method is equivalent to solve the following minimization problem [5,6]:

$$\min_{\mathbf{x}\in\mathbb{R}^n} \varphi(\mathbf{x}) = \min_{\mathbf{x}\in\mathbb{R}^n} \left[\frac{1}{2}\mathbf{x}^{\mathrm{T}}\mathbf{Bx} - \mathbf{b}^{\mathrm{T}}\mathbf{x}\right], \tag{2}$$

where $\mathbf{B}$ is a positive definite matrix.

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

$$\mathbf{r}_0 = \mathbf{b} - \mathbf{Bx}_0. \tag{3}$$

Upon letting

$$\mathbf{z} = \mathbf{x} - \mathbf{x}_0. \tag{4}$$

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Eq. (1) is equivalent to

$$\mathbf{Bz} = \mathbf{r}_0, \tag{5}$$

which can be used to search a descent direction $\mathbf{z}$ after giving an initial residual $\mathbf{r}_0$. Liu [7,8] has proposed by minimizing the following merit function:

$$\min \left\{ a_0 = \frac{\|\mathbf{r}_0\|^2 \|\mathbf{Bz}\|^2}{[\mathbf{r}_0 \cdot (\mathbf{Bz})]^2} \right\}, \tag{6}$$

to obtain a fast descent direction $\mathbf{z}$ in the iterative solution of Eq. (1).

In the numerical solution of linear equations system the Krylov subspace method is one of the most important classes of numerical methods [9–13]. The iterative algorithms that are applied to solve large scale linear systems are mostly the preconditioned Krylov subspace methods [14]. Instead of the development of numerical methods, we will employ the Krylov subspace method to derive a closed-form double optimal solution of Eq. (1) when $\mathbf{B}$ is a non-sparse matrix.

Suppose that we have an m-dimensional Krylov subspace generated by the coefficient matrix $\mathbf{B}$ from the right-hand side vector $\mathbf{r}_0$ in Eq. (5):

$$\mathcal{K}_m := \text{Span}\{\mathbf{r}_0, \mathbf{Br}_0, \ldots, \mathbf{B}^{m-1}\mathbf{r}_0\}. \tag{7}$$

Let $\mathcal{L}_m = \mathbf{B}\mathcal{K}_m$. The idea of GMRES is using the Galerkin method to search the solution $\mathbf{z} \in \mathcal{K}_m$, such that the residual $\mathbf{b} - \mathbf{Bx} = \mathbf{r}_0 - \mathbf{Bz}$ is perpendicular to $\mathcal{L}_m$ [15]. It can be shown that the solution $\mathbf{z} \in \mathcal{K}_m$ minimizes the residual [16]:

$$\min\{\|\mathbf{r}_0 - \mathbf{Bz}\|^2 = \|\mathbf{b} - \mathbf{Bx}\|^2\}. \tag{8}$$

To the best knowledge of the author, there exists no theory and no numerical method to find the solution of Eq. (1), simultaneously based on the two minimizations in Eqs. (6) and (8). The remaining parts of this paper are arranged as follows. In Section 2 we start from an m-dimensional Krylov subspace to express the solution in an affine $m + 1$-dimensional linear subspace with some coefficients to be optimized in Section 3, where two merit functions are proposed for the optimizations of the expansion coefficients. More importantly, we can derive a closed-form double optimal solution (DOS) of Eq. (1). Some important properties of DOS are identified in this section. The procedures to find the DOS are sketched in Section 4. The examples of linear problems, including large scale problems, solved by the method of DOS are given in Section 5 to display some advantages of the present methodology to find approximate solution of Eq. (1). Finally, the conclusions are drawn in Section 6.

2. An affine Krylov subspace method

For the linear equations system (1), by using the Cayley–Hamilton theorem we can expand $\mathbf{B}^{-1}$ by

$$\mathbf{B}^{-1} = \frac{a_1}{a_0}\mathbf{I}_n + \frac{a_2}{a_0}\mathbf{B} + \frac{a_3}{a_0}\mathbf{B}^2 + \cdots + \frac{a_{n-1}}{a_0}\mathbf{B}^{n-2} + \frac{1}{a_0}\mathbf{B}^{n-1}, \tag{9}$$

and hence, the solution $\mathbf{x}$ is given by

$$\mathbf{x} = \mathbf{B}^{-1}\mathbf{b} = \left[\frac{a_1}{a_0}\mathbf{I}_n + \frac{a_2}{a_0}\mathbf{B} + \frac{a_3}{a_0}\mathbf{B}^2 + \cdots + \frac{1}{a_0}\mathbf{B}^{n-1}\right]\mathbf{b}, \tag{10}$$

where the coefficients $a_0, a_1, \ldots, a_{n-1}$ are appeared in the characteristic equation for $\mathbf{B}$: $\lambda^n + a_{n-1}\lambda^{n-1} + \cdots + a_2\lambda^2 + a_1\lambda - a_0 = 0$. Here, we assume that $a_0 = -\det(\mathbf{B}) \neq 0$. In practice, the above formula to find the solution of $\mathbf{x}$ is quite difficult to be realized, since the coefficients $a_j,\ j = 0, 1, \ldots, n-1$ are hard to find, and the computations of the higher-order powers of $\mathbf{B}$ are expansive, when n is a quite large positive integer.

However, motivated by Eq. (10) we can suppose that the solution $\mathbf{x}$ can be expressed by

$$\mathbf{x} = \alpha_0\mathbf{b} + \sum_{k=1}^{m} \alpha_k \mathbf{u}_k, \tag{11}$$

which is to be determined as an optimal combination of $\mathbf{b}$ and the m-vector $\mathbf{u}_k,\ k = 1, \ldots, m$ in an $m + 1$-dimensional linear subspace, when the coefficients α_k and α_0 are optimized in Section 3. For finding the solution $\mathbf{x}$ in a much smaller subspace we suppose that $m \ll n$.

Now we describe how to set up the m-vector $\mathbf{u}_k,\ k = 1, \ldots, m$ by the Krylov subspace method. Suppose that we have an m-dimensional Krylov subspace generated by the coefficient matrix $\mathbf{B}$ from the right-hand side vector $\mathbf{b}$ in Eq. (1):

$$\mathcal{K}_m := \text{Span}\{\mathbf{Bb}, \ldots, \mathbf{B}^m\mathbf{b}\}. \tag{12}$$

Then the Arnoldi process is used to normalize and orthogonalize the Krylov vectors $\mathbf{B}^j\mathbf{b},\ j = 1, \ldots, m$, such that the resultant vectors $\mathbf{u}_i,\ i = 1, \ldots, m$ satisfy $\mathbf{u}_i \cdot \mathbf{u}_j = \delta_{ij},\ i, j = 1, \ldots, m$, where δ_{ij} is the Kronecker delta symbol.