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A NUMERICALLY STABLE BLOCK MODIFIED GRAM-SCHMIDT ALGORITHM FOR SOLVING STIFF WEIGHTED LEAST SQUARES PROBLEMS *

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Abstract

Recently, Wei in [18] proved that perturbed stiff weighted pseudoinverses and stiff weighted least squares problems are stable, if and only if the original and perturbed coefficient matrices A and $\overline{A}$ satisfy several row rank preservation conditions. According to these conditions, in this paper we show that in general, ordinary modified Gram-Schmidt with column pivoting is not numerically stable for solving the stiff weighted least squares problem. We then propose a row block modified Gram-Schmidt algorithm with column pivoting, and show that with appropriately chosen tolerance, this algorithm can correctly determine the numerical ranks of these row partitioned sub-matrices, and the computed QR factor $\overline{R}$ contains small roundoff error which is row stable. Several numerical experiments are also provided to compare the results of the ordinary Modified Gram-Schmidt algorithm with column pivoting and the row block Modified Gram-Schmidt algorithm with column pivoting.

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Key words: Weighted least squares, Stiff, Row block MGS QR, Numerical stability, Rank preserve.

1. Introduction

In this paper, we use the following notations. $\Re^{m\times n}$ is the set of all $m\times n$ matrices with real entries, $\Re_r^{m\times n}$ is a subset of $\Re^{m\times n}$ in which any matrix has rank r. For a given matrix A, A^T is the transpose of A. I and 0 respectively denote the identity and zero matrices with appropriate sizes, e_k is the kth column of the identity matrix I,$e=[1,\cdots,1]$ is a vector with appropriate size, $\|\cdot\|\equiv\|\cdot\|_2$ is the Euclidean vector norm or corresponding subordinate matrix norm. The line over a quantity is the corresponding a perturbed version.

We are concerned with the numerical computations of the stiff weighted least squares (stiff WLS) problem

$$\min_{x\in\Re^n}\|W^{\frac{1}{2}}(Ax-b)\|=\min_x\|D(Ax-b)\|,\tag{1}$$

where $A\in R^{m\times n}, b\in R^m$ are a known coefficient matrix and observation vector, respectively, and

$$D=\operatorname{diag}(d_{11},d_{22},\cdots,d_{mm})=\operatorname{diag}(w_{11}^{\frac{1}{2}},w_{22}^{\frac{1}{2}},\cdots,w_{mm}^{\frac{1}{2}})=W^{\frac{1}{2}}\tag{2}$$

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is the weight matrix in which the scalar parameters $d_1, \cdots, d_m$ vary widely in size. The stiff WLS problem (1) is widely used, e.g., in electronic networks, certain classes of finite element problems, the interior point method for constrained optimization (e.g., see [12]), and for solving the equality constrained least squares problem (e.g., see [1, 13, 14]),

$$\min_{x\in\Re^n} \|Kx - g\| \quad \text{s.t.} \quad Lx = h,$$

by the method of weighting,

$$\min_x \left\| \begin{pmatrix} \tau L \\ K \end{pmatrix} x - \begin{pmatrix} \tau h \\ g \end{pmatrix} \right\|,$$

where τ is a large parameter; one usually chooses $\tau \sim u^{-\frac{1}{2}}$ with u the machine roundoff unit.

The upper bound and the stability of weighted pseudoinverses and WLS problems are very important subjects in areas like numerical linear algebra and optimization, especially after the appearance of the famous paper of Karmarkar [8] which introduced the interior point method for solving optimization problems. The authors of [11, 10, 15, 16, 6] studied the supremum of the weighted pseudoinverses.

Wei [15, 16], Wei and De Pierro [19] proved that when W ranges over $\mathcal{D}$ that is a set of positive definite diagonal matrices, the perturbations are stable to weighted pseudoinverses $A_W^\dagger \equiv (W^{\frac{1}{2}}A)^\dagger W^{\frac{1}{2}}$ and corresponding WLS problems, *if and only if any rank*(A) *rows of the matrix* A *are linearly independent.*

In practical scientific computations, the above condition is too restrictive to hold, and the weight matrix W is usually fixed and severely stiff. In [17], Wei found that the stiff weighted pseudoinverse is close to a related multi-level constrained pseudoinverse $A_C^\dagger$ and the solution set of Eq. (1) is close to a related multi-level constrained least squares problem. Based on this observation, Wei [18] derived the stability conditions of perturbed stiff weighted pseudoinverses and stiff WLS problems.

Without loss of generality, we make the following notation and assumptions for the matrices A and W.

Assumption 1.1. The matrices A and W in Eq. (1) satisfy the following conditions: $\|A(i,:)\|$ have the same order for $i = 1, \cdots, m$, $w_1 > w_2 > \cdots > w_k > 0$, $m_1 + m_2 + \cdots + m_k = m$, and we denote $W = \mathrm{diag}(w_1 I_{m_1}, w_2 I_{m_2}, \cdots, w_k I_{m_k})$,

$$A = \begin{pmatrix} A_1 \\ \vdots \\ A_k \end{pmatrix} \begin{matrix} m_1 \\ \vdots \\ m_k \end{matrix}, \quad C_j = \begin{pmatrix} A_1 \\ \vdots \\ A_j \end{pmatrix}, \quad j = 1, \cdots, k,$$

and assume

$$0 < \epsilon_{ij} \equiv w_i/w_j \ll 1, \text{ for } 1 \le j < i \le k \text{ so } \epsilon = \max_{1\le j<k} \{\epsilon_{j+1,j}\} \ll 1.$$

We also set

$$P_0 = I_n, \quad P_j = I - C_j^\dagger C_j, \quad \mathrm{rank}(C_j) = r_j, \quad j = 1, \cdots, k.$$

With above mentioned matrices A, A_j, C_j and the parameters ϵ_{ij}, denote $\overline{A}$, $\overline{A}_j$, $\overline{C}_j$, $\overline{\epsilon}_{ij}$ as the perturbed versions of A, A_j, C_j, ϵ_{ij}, respectively. Then Wei (in Theorems 3.1–3.5, 4.1-4.2 of [18]) proved the following results.