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A flexible condition number for weighted linear least squares problem and its statistical estimation☆

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ABSTRACT

In this paper, we mainly focus on the derivation of a flexible condition number for weighted linear least squares problem and its estimation. With Fréchet derivative and Kronecker product, the explicit expression of the condition number is obtained. When the coefficient matrices are large and dense, considering the difficulties of explicitly forming the expression of condition number in computer, we also present its simplified form through a simple and easy to operate method. Two different condition estimation methods are introduced, and the numerical experiments are also performed to show the efficiency of the condition estimators.

1. Introduction

The precise definition of condition number may be first given by Rice in [1], which is treated as the maximum amplification of the resulting change in solution with respect to a perturbation in the data. In [2], Geurts presented another equivalent definition of condition number, and regularized the use of condition number by establishing the equalities and specifying the norms. In this paper, we would like to follow the regulations given by Geurts. Suppose that f is a map from the data space $\mathbb{R}^m$ to the solution space $\mathbb{R}^n$, and $\mathbb{R}^m$ and $\mathbb{R}^n$ are equipped with the norms $\|\cdot\|_{\mathcal{D}}$ and $\|\cdot\|_{\mathcal{S}}$ respectively. Then the absolute condition number of f at $x_0 \in \mathbb{R}^m$ is defined as

$$\kappa_f(x_0) = \lim_{\delta\to 0} \sup_{0<\|x-x_0\|_{\mathcal{D}}\leqslant\delta} \frac{\|f(x)-f(x_0)\|_{\mathcal{S}}}{\|x-x_0\|_{\mathcal{D}}}, \tag{1.1}$$

and the relative condition number is given by

$$\kappa_f^{rel}(x_0) = \frac{\kappa_f(x_0)\|x_0\|_{\mathcal{D}}}{\|f(x_0)\|_{\mathcal{S}}},$$

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which is exactly the one given by Geurts. When f is Fréchet differentiable, from [2] we have

$$\kappa_f(x_0) = \|Df(x_0)\|_{\mathcal{D}\mathcal{S}}, \quad \text{and} \quad \kappa_f^{rel}(x_0) = \frac{\|Df(x_0)\|_{\mathcal{D}\mathcal{S}}\|x_0\|_{\mathcal{D}}}{\|f(x_0)\|_{\mathcal{S}}},$$

where $Df(x_0)$ denotes the Fréchet derivative of f at x_0, and $\|\cdot\|_{\mathcal{D}\mathcal{S}}$ is the operator norm induced by $\|\cdot\|_{\mathcal{D}}$ and $\|\cdot\|_{\mathcal{S}}$. With singular value decomposition, Geurts [2] established the explicit expression of the condition number for linear least squares (LLS) problem $\min_x \|Ax - b\|_2$ without considering perturbation to b. In [3], considering the perturbations to both A and b, Gratton proposed a condition number of LLS problem by putting the weighted Frobenius norm $\|[\alpha A, \beta b]\|_F$ $(\alpha, \beta > 0)$ on the data space and the Euclidean norm on the solution space, and presented its explicit expression. A more general weighted Frobenius norm $\|[AT, \beta b]\|_F$ with T being a positive definite diagonal matrix (generally, T can be any positive definite matrix, but there is no loss of generality to assume that T is diagonal, since the positive definite matrix can be diagonalized with unitary transformation) was given by Wei et al. [4] in deriving the explicit expression of the condition number for rank deficient LLS problem. It has been shown in [3–5] that the weighted Frobenius norm makes the condition number to preserve the flexibility in the sense that varying the parameters T and β will produce the condition number of LLS problem with respect to A or b, and then we may call this kind of condition number the flexible condition number.

This paper is intended to derive the explicit expression of the flexible condition number and its statistical estimation for the weighted linear least squares (WLLS) problem

$$\min_{x\in\mathbb{R}^n} \|Ax - b\|_M, \tag{1.2}$$

where $A \in \mathbb{R}^{m\times n}$ has full column rank, $b \in \mathbb{R}^m$, and $\|\cdot\|_M$ is the weighted vector M-norm [6, p. 27]. Here, we consider the WLLS problem with minimal N-norm solution $\|x\|_N$ (see [7]). The condition number of WLLS problem has been studied by many researchers. With the restrictions $R(\Delta A) \subseteq R(A)$ and $R(\Delta A^T) \subseteq R(A^T)$ on the perturbation, Wei et al. [8] studied the explicit normwise condition numbers of weighted Moore–Penrose (WMP) inverse and WLLS problem. Wang et al. [9] reconsidered relaxing this condition. In [10], Li et al. derived the explicit expressions of mixed and componentwise condition numbers of WMP inverse and WLLS problem. For more details on WLLS problem see [7,11,12] and references therein.

The main contribution of this paper is that by the Fréchet derivative and Kronecker product, we establish the explicit expression of the flexible condition number, and give its simplified form through the techniques used in [13]. One can find that the approach used in this paper is easy to operate and needs little constructive techniques. We also show that if the weighted singular value decomposition is available, the expression of flexible condition number can be reduced to the same form as the one given by Gratton in [3]. In addition, we devise two different algorithms to estimate the condition number, and use random numerical WLLS problems to check the efficiency of the condition estimators.

The rest of the paper is organized as follows. Section 2 contains some preliminaries and useful results. In Section 3, we carry out the derivation of the explicit expression of the condition number and its simplification. Section 4 is devoted to the numerical experiments. A concluding remark is given in Section 5.

2. Notation and preliminaries

Let I_n be the identity matrix of order n. The symbols A^T, $\|A\|_2$, and $\|A\|_F$ denote the transpose, spectral norm, and Frobenius norm of matrix A, respectively. Then, we present some basic concepts which will be used throughout the paper. The weighted inner products in $\mathbb{R}^m$ and $\mathbb{R}^n$ are defined by

$$(x, y)_M = y^T Mx, \quad x, y \in \mathbb{R}^m, \quad \text{and} \quad (x, y)_N = y^T Nx, \quad x, y \in \mathbb{R}^n,$$

with $M \in \mathbb{R}^{m\times m}$ and $N \in \mathbb{R}^{n\times n}$ being positive definite matrices. The corresponding definitions of weighted vector norms are given by

$$\|x\|_M = (x, x)_M^{\frac{1}{2}} = (x^T Mx)^{\frac{1}{2}} = \left\|M^{\frac{1}{2}}x\right\|_2, \quad x \in \mathbb{R}^m,$$

and

$$\|x\|_N = (x, x)_N^{\frac{1}{2}} = (x^T Nx)^{\frac{1}{2}} = \left\|N^{\frac{1}{2}}x\right\|_2, \quad x \in \mathbb{R}^n.$$

For a matrix $A \in \mathbb{R}^{m\times n}$, the weighted matrix norm of A is defined by

$$\|A\|_{MN} = \max_{\|x\|_N=1} \|Ax\|_M, \quad x \in \mathbb{R}^n.$$

Similarly, for $B \in \mathbb{R}^{n\times m}$, we have

$$\|B\|_{NM} = \max_{\|x\|_M=1} \|Bx\|_N, \quad x \in \mathbb{R}^m.$$

It is easy to verify that

$$\|A\|_{MN} = \left\|M^{\frac{1}{2}}AN^{-\frac{1}{2}}\right\|_2, \quad \text{and} \quad \|B\|_{NM} = \left\|N^{\frac{1}{2}}BM^{-\frac{1}{2}}\right\|_2. \tag{2.1}$$