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Solving Least Squares Problems With Equality Constraints Based On Augmented Regularized Normal Equations*

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Abstract

This article is devoted to a new algorithm for solving least squares problems with linear equality constraints. The presented algorithm can help solve large dimension ill-conditioned problems efficiently.

1 Statement of the Problem

The considered least squares problem with linear equality constraints (LSE) is given by

$$\min_{Bx=d} \|Ax - b\|_2, \tag{1}$$

where $A \in \mathbb{R}^{m\times n}$, $B \in \mathbb{R}^{p\times n}$, $b \in \mathbb{R}^m$, $d \in \mathbb{R}^p$, $\operatorname{rank}(B) = p < n$, and $\|\cdot\|_2$ is the Euclidean norm.

The LSE problem is significant for applied regression analysis, which is one of the universal methods for modern mathematical modeling. Regression analysis is widely used in econometric problems solving.

In [1] it is noted that the method of Lagrange multipliers is inefficient for this problem, therefore two other approaches are proposed.

The first approach is based on orthogonal transformations (QR decomposition using Householder and Givens transformations). However, this approach has a high computational complexity and is numerically less stable if A and B are ill-conditioned matrices, which significantly reduces the practical application of this approach.

The second approach is to obtain an approximate solution of problem (1) based on the least squares problem without constraints:

$$\min_{x\in\mathbb{R}^n} \left\| \begin{pmatrix} A \\ \lambda B \end{pmatrix} x - \begin{pmatrix} b \\ \lambda d \end{pmatrix} \right\|_2 \tag{2}$$

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for large λ ($\lambda \gg 1$).

The problem (2) is equivalent to the weighted least squares problem

$$\min_{x\in\mathbb{R}^n} \|D_\lambda(Fx-g)\|_2, \tag{3}$$

where

$$F = \begin{pmatrix} A \\ B \end{pmatrix} \in \mathbb{R}^{(m+p)\times n}, \qquad g = \begin{pmatrix} b \\ d \end{pmatrix} \in \mathbb{R}^{m+p},$$

and

$$D_\lambda = \operatorname{diag}(\underbrace{1,\dots,1}_{m},\underbrace{\lambda,\dots,\lambda}_{p}).$$

In [2] the analysis based on the generalized singular value decomposition (GSVD) was conducted to determine the quality of the approximation (corresponding to the solution of the weighted least squares problem (3)) to the solution of the initial LSE problem (1).

Suppose $m \geq n$ and

$$U^\top AX = \operatorname{diag}(\alpha_1,\dots,\alpha_n) = D_A \in \mathbb{R}^{m\times n},$$

$$V^\top BX = \operatorname{diag}(\beta_1,\dots,\beta_p) = D_B \in \mathbb{R}^{p\times n}$$

form the GSVD of two matrices (A, B), where $^\top$ denotes the transpose. We will assume (without loss of generality) that both matrices A and B have full rank. If

$$U = [u_1,\dots,u_m], \quad V = [v_1,\dots,v_p], \quad X = [x_1,\dots,x_n],$$

from GSVD, it directly follows that

$$x_* = \sum_{i=1}^{p} \frac{v_i^\top d}{\beta_i} x_i + \sum_{i=i+1}^{n} \frac{u_i^\top b}{\alpha_i} x_i \tag{4}$$

is the exact solution of the LSE problem (1), whereas

$$x(\lambda) = \sum_{i=1}^{p} \frac{\alpha_i u_i^\top b + \lambda^2\beta_i^2 v_i^\top d}{\alpha_i^2+\lambda^2\beta_i^2} + \sum_{i=i+1}^{n} \frac{u_i^\top b}{\alpha_i} x_i \tag{5}$$

is the solution of the weighted least squares problem (3).

Then from (4) and (5), we obtain

$$x(\lambda) - x_* = \sum_{i=1}^{p} \frac{\alpha_i u_i^\top b + \lambda^2\beta_i^2 v_i^\top d}{\alpha_i^2+\lambda^2\beta_i^2} - \sum_{i=1}^{p} \frac{v_i^\top d}{\beta_i} x_i = \sum_{i=1}^{p} \frac{\alpha_i(\beta_i u_i^\top b - \alpha_i v_i^\top d)}{\beta_i(\alpha_i^2+\lambda^2\beta_i^2)}$$

and, therefore

$$\lim_{\lambda\to\infty} \|x(\lambda) - x_*\|_2 = 0.$$

As noted in [1], the appeal of the way to obtain the approximate solution of the LSE problem (1) using the weighted least squares method is that special subprograms are not required: only subprograms for solving ordinary normal equations (6) are used

$$F^\top D_\lambda^2 F x = F^\top D_\lambda g \quad \Longleftrightarrow \quad (A^\top A + \lambda^2 B^\top B)x = A^\top b + \lambda^2 B^\top d. \tag{6}$$

However, for large values of the parameter λ, the matrix $F^\top D_\lambda^2 F$ of the normal system (6) becomes extremely ill-conditioned and, as a result, its solving is numerically unstable when performing calculations on the computer with floating-point arithmetic.

2 Method of Augmented Regularized Normal Equations

Suppose that t bit floating-point arithmetic with the base ν is used and the parameter λ is defined as $\lambda = 10^r$. Thus, if $\lambda^2 = 10^{2r} \geq \nu^t$, then for the solutions $\tilde{x}(\lambda)$ of normal equations (6), we cannot guarantee any correct significant figure in the computed solution. However, as it is shown above, having a higher value of the parameter λ, we obtain more accurate solution of weighted least squares problem (3).

In this paper we present a new approach for solving the problem (2) based on augmented regularized normal equations [2].

The method of augmented regularized normal equations proposed in [2] is based on the following facts.

First, it was shown in [2] that the regularized normal equations problem solving (the Euler equations)

$$(F^T F + \alpha E_s)x = F^T g \tag{7}$$

is equivalent to solving the augmented regularized normal equations problem

$$\begin{pmatrix} \omega E_r & F \\ F^T & -\omega E_s \end{pmatrix} \begin{pmatrix} y \\ x \end{pmatrix} = \begin{pmatrix} g \\ 0 \end{pmatrix}, \tag{8}$$

where $F \in \mathbb{R}^{r \times s}$, $g \in \mathbb{R}^r$, $\alpha > 0$ is a regularization parameter, E_r and E_s are identity matrices of orders r and s respectively, $y = \omega^{-1}\mu$, $\mu = g - Fx$, $\omega = \alpha^{1/2}$.

Second, it was shown in [2] that the spectral condition numbers of augmented regularized normal equations matrix (8) and ordinary regularized normal equations matrix (7) are related as follows:

$$\operatorname{cond}_2 \begin{pmatrix} \omega E_r & F \\ F^T & -\omega E_s \end{pmatrix} = \sqrt{\operatorname{cond}_2(F^T F + \alpha E_s)}.$$

This fact gives significant advantages of augmented regularized normal equations (8) over ordinary regularized normal equations (7). The method based on the augmented regularized normal equations (8) can be used for the numerically stable calculation of pseudosolutions for rank-deficient system of linear algebraic equations $Fx = g$ or for systems of linear algebraic equations that are numerically rank-deficient.

This approach is based on the following well-known fact: since $\alpha \to 0$, the solution x_α for system (7) tends to the normal pseudosolution

$$x_* = F^+ g, \tag{9}$$

where F^+ is a pseudoinverse matrix. Consequently, the solution x_ω of augmented system (8) also converges to pseudosolution (9) if $\omega \to 0$.

Let the floating-point arithmetic with p digits and base β be used for calculations. Then the application of augmented normal equations (8) makes it possible to obtain a significantly more accurate approximation to pseudosolution (9) compared to the approximation provided by normal equations (7) in the same arithmetic.

Suppose that the parameter ω is chosen to obey the conditions $\omega^2 \le \eta$ and $\omega > \eta$, where $\eta = \beta^{-p}$. Then, to machine precision, the matrices $F^T F + \omega^2 E_s$ and $F^T F$ are equal. In addition, we require that the choice of ω minimize the condition number of augmented system (8). In accordance with these requirements, we set

$$\omega = \omega_* = 10^{-q}, \tag{10}$$

where $q = \min\{k \in \mathbb{N} : 10^{-2k} \le \eta\}$. Consequently, the choice of ω in the form of (10) ensures that the condition

$$\min_{\omega^2 \le \eta} \operatorname{cond}_2 \begin{pmatrix} \omega E_r & F \\ F^T & -\omega E_s \end{pmatrix}$$

is fulfilled on the set $\{10^{-k} : k \in \mathbb{N}\}$. If the machine precision $\eta \approx 10^{-d}$, then $q \approx d/2$. In MatLab, we have $d = 17$. The above mentioned choice of ω corresponds to $q = 9$, which gives $\omega_* = 10^{-9}$.

This approach allows us to solve the problem (2) at much higher values of the parameter λ compared with the method based on the weighted normal equations (6), when performing calculations in the same t-bit floating-point arithmetic with the base ν. Therefore, the proposed approach provides a much more accurate approximation to the solution of the original least squares problem with linear equality constraints (1). It is obvious that the solution of (2) can be given by

$$x(\lambda) = \begin{pmatrix} A \\ \lambda B \end{pmatrix}^+ \begin{pmatrix} b \\ \lambda d \end{pmatrix}, \tag{11}$$

where $(\cdot)^+$ is a Moore-Penrose pseudoinverse of a matrix [3].

For large values λ, the matrix $\begin{pmatrix} A \\ \lambda B \end{pmatrix}$ is extremely ill-conditioned and the solution of the corresponding system of linear algebraic equations causes serious computational difficulties. For solving (7), the method of augmented regularized normal equations considered above is proposed. In (8), if we suppose $F = F_\lambda$, $g = g_\lambda$ and respectively $r = m+p$, and $s = n$, then, according to this method, the solution $x(\lambda)$ is defined from system

$$\begin{pmatrix} \omega E_{m+p} & F_\lambda \\ F_\lambda^\top & -\omega E_n \end{pmatrix} \begin{pmatrix} y \\ x \end{pmatrix} = \begin{pmatrix} g_\lambda \\ 0 \end{pmatrix}, \tag{12}$$

where E_{m+p} and E_n are identity matrices of orders $m+p$ and n respectively,

$$F_\lambda = \begin{pmatrix} A \\ \lambda B \end{pmatrix} \in \mathbb{R}^{(m+p)\times n} \quad \text{and } g_\lambda = \begin{pmatrix} b \\ \lambda d \end{pmatrix} \in \mathbb{R}^{m+p}.$$

The parameter ω, in accordance with [2], is defined as $\omega = 10^{-q}$ where

$$q = \min\{k \in \mathbb{N} : 10^{-2k} \le \nu^{-t}\},$$

and $\lambda = 10^q$.

As it was shown in [2], the values $\omega = 10^{-6}$ and $\lambda = 10^6$ correspond to calculations with single precision, and $\omega = 10^{-9}$ and $\lambda = 10^9$ are predefined for MatLab.

This approach allows to solve (with high precision) LSE problems efficiently. In this case, it does not require development of specific programs as obtaining a solution is reduced to solving a system of linear algebraic equations (12) using any standard program.

3 Numerical Experiment

The effectiveness of the proposed approach is illustrated by a simple test case. Consider the LSE problem:

$$\min_{x_1+x_2=1} \left\| \begin{pmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} - \begin{pmatrix} 7 \\ 1 \\ 3 \end{pmatrix} \right\|_2 . \tag{13}$$

For the problem (13), we can easily calculate the exact solution vector $x_* = (x_{*1}, x_{*2})^\top$, which allows to use (13) to test the proposed approach for solving arbitrary LSE problems.

We express x_2 as a function of x_1, then $x_2 = 1 - x_1$ and the problem (13) can be transformed to an ordinary least squares problem without constraints (with one variable):

$$\min_{x_1\in\mathbb{R}} \left\| \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} x_1 - \begin{pmatrix} -5 \\ 3 \\ 3 \end{pmatrix} \right\|_2 . \tag{14}$$

It is obvious that the solution of (14) is $x_{*1} = 1/3$ and therefore, the solution of LSE problem (13) is $x_* = (1/3, 2/3)^\top$.

Further we shall deal with the solving of the problem (13) using the augmented regularized normal equations (12). For the problem (13), we have $m = 3$ and $p = 1$. Let $\lambda = 10^6$. Then

$$F_\lambda = \begin{pmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \\ 10^6 & 10^6 \end{pmatrix}, \quad g_\lambda = \begin{pmatrix} 7 \\ 1 \\ 3 \\ 10^6 \end{pmatrix},$$

and the corresponding augmented normal system (12) is consistent and has order $m + p + n = 6$. For this example, the augmented regularized normal equations have the form of

$$\begin{pmatrix} \omega & 0 & 0 & 0 & 1 & 2 \\ 0 & \omega & 0 & 0 & 3 & 4 \\ 0 & 0 & \omega & 0 & 5 & 6 \\ 0 & 0 & 0 & \omega & 10^6 & 10^6 \\ 1 & 3 & 5 & 10^6 & -\omega & 0 \\ 2 & 4 & 6 & 10^6 & 0 & -\omega \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 7 \\ 1 \\ 3 \\ 10^6 \\ 0 \\ 0 \end{pmatrix}, \tag{15}$$

where the parameter ω is chosen according to the digit capacity of the floating-point arithmetic. The system (15) is solved using the Crout method (modification of the Gaussian elimination method) with single precision for $\omega = 10^{-6}$. The following result has been obtained:

$$\hat{x}_1 = 0.33333333328 \ \text{ and } \ \hat{x}_2 = 0.66666666671.$$

At the same time, the Cholesky method for solving ordinary normal equations (3) for $\lambda = 10^6$ shows that

$$\hat{x}_1 = 0.19999999999 \ \text{ and } \ \hat{x}_2 = 0.80000000000.$$

Consider the second example that illustrates a possibility of solving the problem using the proposed method for:

$$\text{rank} \begin{pmatrix} A \\ B \end{pmatrix} < n.$$

The LSE problem:

$$\min_{x_1+x_2=3} \left\| \begin{pmatrix} 1 & 2 \\ 2 & 4 \\ 3 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} - \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \right\|_2 . \tag{16}$$

The solution of LSE problem (16) is $x_* = (0.6, 1.2)^\top$.

Further we shall deal with the solving of the problem (16) using the augmented regularized normal equations (12). For the problem (16), we have $m = 3$ and $p = 1$. Let $\lambda = 10^6$, then

$$F_\lambda = \begin{pmatrix} 1 & 2 \\ 2 & 4 \\ 3 & 6 \\ 10^6 & 10^6 \end{pmatrix}, \quad g_\lambda = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 10^6 \end{pmatrix},$$

and the corresponding augmented normal system (12) is consistent and has order $m + p + n = 6$. For this example, the augmented regularized normal equations have the form of

$$\begin{pmatrix} \omega & 0 & 0 & 0 & 1 & 2 \\ 0 & \omega & 0 & 0 & 2 & 4 \\ 0 & 0 & \omega & 0 & 3 & 6 \\ 0 & 0 & 0 & \omega & 10^6 & 10^6 \\ 1 & 2 & 3 & 10^6 & -\omega & 0 \\ 2 & 4 & 6 & 10^6 & 0 & -\omega \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 10^6 \\ 0 \\ 0 \end{pmatrix}. \tag{17}$$

The system (17) is solved using the Crout method with single precision for $\omega = 10^{-6}$. The following result has been obtained:

$$\hat{x}_1 = 0.59999999999 \quad \text{and} \quad \hat{x}_2 = 1.20000000000.$$

4 Conclusion

Thus, the use of ordinary normal equations does not allow to solve the considered problem, whereas the proposed method based on augmented regularized normal equations solves this problem almost accurately. Using double precision and having $\omega = 10^{-12}$ and $\lambda = 10^{12}$, the method based on the augmented regularized normal equations provides a solution accurate to all significant figures.

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