IEICE Proceeding Series

Verified bounds for Least Squares Problems and Underdetermined Linear Systems

Siegfried M. Rump

Vol. 1 pp. 881-882
Publication Date: 2014/03/17
Online ISSN: 2188-5079

2012 International Symposium on Nonlinear Theory and its Applications
NOLTA2012, Palma, Majorca, Spain, October 22-26, 2012

Verified bounds for Least Squares Problems and Underdetermined Linear Systems

Siegfried M. Rump†

†Institute for Reliable Computing,
Hamburg University of Technology,
Schwarzenbergstraße 95, Hamburg 21071, Germany,

and Visiting Professor at Waseda University,
Faculty of Science and Engineering,
3–4–1 Okubo, Shinjuku-ku, Tokyo 169–8555, Japan

Email: rump@tu-harburg.de

1. Main results

We present new algorithms for computing verified error bounds for least squares problems and underdetermined linear systems. In contrast to previous approaches the new methods do not rely on normal equations and are applicable to sparse matrices. This paper summarizes some results; a full paper was published in [7].

Algorithms based on normal equations are available in INTLAB [6]. For an $m \times n$-matrix they require $O([m+n]^3)$ floating-point operations. Therefore, larger problems are not tractable, in particular because the sparsity of the matrices involved cannot be taken advantage of.

For underdetermined linear systems, i.e. $Ax = b$ with $A \in \mathbb{R}^{m\times n}$ and $m < n$, Miyajima [4] proposed a faster algorithm requiring $O(mn^2)$ operations. The challenge is to obtain verified bounds in a computing time proportional to that needed for an approximate solution, namely $O(m^2n)$ operations for underdetermined linear systems and $O(mn^2)$ operations for least squares problems.

Our key to obtain fast algorithms are a number of perturbation bounds. A matrix of floating-point numbers may be nearly orthogonal but is, in general, not truly orthogonal. The distance to orthogonality is estimated by certain lemmas like the following.

Lemma 1 *Let $X \in \mathbb{R}^{m\times n}$ and $p \in \{1,2,\infty\}$ be given, and suppose $\|I - X^TX\|_p \le \alpha < 1$. Then $m \ge n$, X has full rank, and*

$$\|X^+ - X^T\|_2 \le \frac{\alpha}{\sqrt{1-\alpha}} \quad \text{for } p = 2\,. \tag{1}$$

Moreover, for any $B \in \mathbb{R}^{m\times k}$ with $k \ge 1$,

$$\|(X^+ - X^T)B\|_p \le \frac{\alpha\|X^TB\|_p}{1-\alpha} \quad \text{for } p \in \{1,2,\infty\}\,. \tag{2}$$

Lemma 2 *Let $A \in \mathbb{R}^{m\times n}$ and $P \in \mathbb{R}^{n\times m}$ with $m \ge n$ and $p \in \{1,2,\infty\}$ be given, and suppose $\|I - PA\|_p \le \alpha < 1$. Then A and P have full rank, and*

$$\|A^+\|_p \le \frac{\varphi\|P\|_p}{1-\alpha} \tag{3}$$

with $\varphi = 1$ for $p = 2$, and $\varphi = \frac{\sqrt{m}+1}{2}$ for $p \in \{1,\infty\}$.

The new methods basically compute floating-point approximations, and then estimate the error to the true solution based on lemmas as above. A similar technique was used by Miyajima for underdetermined linear systems.

Lemma 3 *(Miyajima [4]) Let $A \in \mathbb{R}^{n\times m}$ with $n < m$, $\widetilde{x} \in \mathbb{R}^m$, $\widetilde{w}, b \in \mathbb{R}^n$, $Q \in \mathbb{R}^{m\times n}$, and $R, S \in \mathbb{R}^{n\times n}$ be given. Assume $\|I - Q^TQ\|_2 \le \mu < 1$ and $\|S(R^TQ^T - A)\|_2 \le \rho < \sqrt{1-\mu}$. Then A has full rank and*

$$\|A^+b - \widetilde{x}\|_2 \le \|\widetilde{x} - A^T\widetilde{w}\|_2 + \frac{\|S(A\widetilde{x} - b)\|_2}{\sqrt{1-\mu} - \rho}\,. \tag{4}$$

The bound can be computed in $6m^2n + 8mn^2 + \frac{10}{3}n^3 + O(m^2)$ operations.

The computing time is proportional to $O(m^2n)$ operations. A verification method requiring only $O(mn^2)$ operations is obtained by the following lemma. If the matrix is not far from square, there is not much difference in computing time; the new method becomes faster in case of many unknowns compared to few constraints.

Lemma 4 *Let $A \in \mathbb{R}^{n\times m}$ with $n < m$, $\widetilde{x} \in \mathbb{R}^m$, $\widetilde{w}, b \in \mathbb{R}^n$, $S \in \mathbb{R}^{n\times n}$, and $p \in \{1,2,\infty\}$ be given. Define $Y := SA$ and suppose $\|I - YY^T\|_p \le \alpha < 1$. Then A has full rank and, abbreviating $\rho_{\widetilde{w}} := \widetilde{x} - A^T\widetilde{w}$ and $\rho_{\widetilde{x}} := A\widetilde{x} - b$,*

$$\|A^+b - \widetilde{x}\|_2 \le \|\rho_{\widetilde{w}}\|_2 + \|Y^TS\rho_{\widetilde{x}}\|_2 + \frac{\alpha}{\sqrt{1-\alpha}}\|S\rho_{\widetilde{x}}\|_2\,. \tag{5}$$

The bounds can be computed in $4mn^2 + \frac{4}{3}n^3 + O(m^2)$ operations.

A similar fast method for least squares problems was not known. In contrast to underdetermined systems, the error of some $\tilde{x}$ to the least squares solution can be bounded knowing only the residual $A\tilde{x} - b$. For a given approximate solution $\widetilde{x}$, Lemma 2 implies for $\|I - PA\|_2 \le \alpha < 1$ the straightforward but pessimistic bound

$$\|A^+ b - \widetilde{x}\|_2 = \|A^+(A^T)^+\rho\|_2 \le [\|P\|_2 1 - \alpha]^2 \, \|\rho\|_2 \, , \quad (6)$$

where $\rho := A^T(A\widetilde{x} - b)$. Note that $\rho = 0$ for the solution $\widetilde{x} = A^+ b$. In general, however, this bound is poor.

The following result is based on an approximate QR-decomposition of A. For S denoting an approximate inverse of R, AS can be expected to be not too far from orthogonality. Note that often $m \gg n$ for $A \in \mathbb{R}^{m\times n}$, so that the computational effort to compute S is not too large compared to that for the QR-decomposition.

Lemma 5 *Let $A \in \mathbb{R}^{m\times n}$ with $m \ge n$, $\widetilde{x} \in \mathbb{R}^n$, $\widetilde{w}, b \in \mathbb{R}^m$, $S \in \mathbb{R}^{n\times n}$, and $p \in \{1, 2, \infty\}$ be given. Define $X := AS$ and suppose $\|I - X^T X\|_p \le \alpha < 1$. Then A has full rank and, abbreviating $\rho_{\widetilde{x}} := A\widetilde{x} - \widetilde{w} - b$ and $\rho_{\widetilde{w}} := A^T\widetilde{w}$,*

$$\|\widetilde{x} - A^+ b\|_p \le \frac{\|S\|_p}{1-\alpha} \cdot \left(\|X^T\rho_{\widetilde{x}}\|_p + \|S^T\rho_{\widetilde{w}}\|_p\right) \qquad (7)$$

for $p \in \{1, 2, \infty\}$. The bounds can be computed in $4mn^2 + \frac{4}{3}n^3 + O(m^2)$ operations.

A main point to improve the accuracy of the error bounds are newly developed residual iterations. In both problems, underdetermined systems and least squares problems, the ill-conditioning of the normal equations appear in the computation of a residual. Thus it is important to compute a residual as accurate as possible.

To this purpose we developed algorithms for accurate computation of dot products, see [5, 8]. Those are based on methods already proposed by [3], which represent the sum or product of two floating-point numbers a, b by the sum of an approximation x and an error term y, i.e. $a + b = x + y$ or $ab = x + y$, respectively. Both equations are satisfied with mathematical equality. Recently those methods are called "error-free transformations" and receive increasing interest [2].

Some computational results for the new algorithms on matrices of the Florida matrix collection [1] are shown in Table 1. The sparsity is between 0.02 and 25%. As can be seen the error bounds are correct up to 12 to 15 decimal digits.

More details and also more test results for underdetermined linear systems and least squares problems as well as comparisons to other existing methods are shown in [7]. The new algorithms are significantly faster than known methods.

Table 1: Median relative error of the bounds and median computing time in seconds for our new algorithm based on Lemma5. The number of rows m, columns n, and name of the test matrix are displayed.

m	n	Test matrix	dig.	time
37932	331	`JGD_Taha/abtaha2`	14.3	3.7
14596	209	`JGD_Taha/abtaha1`	14.4	1.10
29493	11822	`Sumner/graphics`	14.5	654
10595	4929	`HB/gemat1`	12.4	46
12061	2262	`LPnetlib/lp_80bau3b`	14.7	8.4
13525	3000	`LPnetlib/lp_fit2p`	14.9	40.6
25067	1118	`LPnetlib/lp_osa_07`	14.8	11.8
54797	2337	`LPnetlib/lp_osa_14`	14.7	56
23541	16675	`LPnetlib/lp_stocfor3`	12.9	1684
63516	507	`Mittelmann/rail507`	14.5	11.6
10757	124	`Meszaros/air03`	15.2	1.46
16819	4400	`Meszaros/model10`	14.6	41
123409	73	`Meszaros/nw14`	14.1	12.8
61521	4050	`Meszaros/rlfddd`	14.2	88
63076	3173	`Meszaros/stat96v4`	12.0	719
184756	190	`JGD_BIBD/bibd_20_10`	15.0	100
319770	231	`JGD_BIBD/bibd_22_8`	14.8	116

References

[1] T.A. Davis and Y. Hu. The University of Florida Sparse Matrix Collection. *ACM Trans. Math. Softw.*, 38(1):1:1–1:25, 2011.

[2] S. Graillat. Applications of fast and accurate summation in computational geometry. In *Proceedings of the 2006 ACM Symposium on Applied Computing*, number CMS-108, 2006.

[3] D.E. Knuth. *The Art of Computer Programming–Seminumerical Algorithms*, Vol. 2, Addison Wesley, Reading, Massachusetts, 1969.

[4] S. Miyajima. Fast enclosure for solutions in underdetermined systems. *J. Comput. Appl. Math.*, 234:3436–3444, 2010.

[5] T. Ogita, S.M. Rump, and S. Oishi. Accurate sum and dot product. *SIAM J. Sci. Comput.*, 26(6):1955–1988, 2005.

[6] S.M. Rump. INTLAB - Interval Laboratory, Version 6. `http://www.ti3.tu-harburg.de/rump`, 1998–2012.

[7] S.M. Rump. Verified Bounds for Least Squares Problems and Underdetermined Linear Systems. *SIAM J. Matrix Anal. Appl. (SIMAX)*, 33(1):130–148, 2012.

[8] S.M. Rump, T. Ogita, and S. Oishi. Accurate floating-point summation part I: Faithful rounding. *SIAM J. Sci. Comput.*, 31(1):189–224, 2008.