

## Pete Stewart's contributions to least-squares backward errors

Commentary by Michael Saunders

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Pete's lifelong interest in backward errors for least-squares problems has greatly influenced one part of scientific computing that some of us are concerned with. His 1977 paper related to LINPACK [6] presented a computable estimate of the backward error for an approximate solution to  $\min \|b - Ax\|$ . This led to a practical method for terminating the iterative solver LSQR [2].

In 1975, Pete had published a little-known result in the SIGNUM Newsletter [5]. Let  $\hat{x}$  and  $\hat{r} = b - A\hat{x}$  be the exact least-squares solution and residual. Pete showed that any *approximate* solution  $x$  with residual  $r = b - Ax$  is the exact least-squares solution of the perturbed problem  $\min \|b - (A + E_1)x\|$ , where  $E_1$  is the rank-one matrix

$$E_1 = \frac{ex^T}{\|x\|^2}, \quad \|E_1\| = \frac{\|e\|}{\|x\|},$$

with  $e \equiv r - \hat{r}$  and  $\|r\|^2 = \|\hat{r}\|^2 + \|e\|^2$ . Of course we normally don't know the exact  $\|\hat{r}\|$ , but Pete noted an important insight—that if  $\|r\|$  is close to the minimum possible value (when  $\|e\|$  is small), it is futile to search for an improved solution because  $x$  already solves a problem with  $A$  only slightly perturbed. (Recall that iterative solvers tend to reach accurate values of  $\|r\|$  and hence small  $\|e\|$  long before  $x$  settles down.)

Soon after, Pete's 1977 paper gave a further important result that can be used within any least-squares solver. The same  $x$  and  $r$  are also the exact least-squares solution of the perturbed problem  $\min \|b - (A + E_2)x\|$ , where  $E_2$  is the rank-one matrix

$$E_2 = -\frac{rr^T A}{\|r\|^2}, \quad \|E_2\| = \frac{\|A^T r\|}{\|r\|}.$$

Luckily Chris Paige knew of Pete's result and showed how to use it within the stopping rule that LSQR uses for least-squares problems. (At each iteration, the current  $\|r\|$  and  $\|A^T r\|$  can be accurately estimated at essentially no cost.) This rule has served us well for nearly 30 years. We thank Pete for making it possible.

To emphasize the significance of  $E_1$  and  $E_2$ , I want to comment that neither backward error is especially easy to confirm even when we know the answer. It took me several hours one day to verify both results, so I doubt that they are fair questions for PhD qualifying exams. (Admittedly the 2009 US Open Tennis streaming video was showing on my Mac at the time!) In optimization, we may confirm reasonably easily that a given constrained optimization problem is the dual of a given primal problem (by showing that the KKT conditions are the same for each problem), but to derive the dual in the first place is a far greater challenge. We can only wonder how Pete managed to derive  $E_1$  and  $E_2$  without knowing in advance that such rank-one matrices exist.

Note that  $\|A^T r\|/\|r\|$  can vary dramatically during the LSQR iterations. Empirically it seems to be 100 to 10,000 times as large as the *optimal* backward error at each stage. Hence the search continues for improved backward-error estimates and more reliable stopping rules.

In the case of dense matrices, Pete himself is leading the way. Suppose  $A$  is  $m \times n$ . For inconsistent LS problems, the optimal backward error norm

$$\mu(x) \equiv \min_E \|E\| \quad \text{s.t.} \quad (A + E)^T(A + E)x = (A + E)^T b$$

is known to be the smallest singular value of a certain  $m \times (n + m)$  matrix  $C$ ; see Waldén et al. [9] and Higham [1, pp. 392–393]:

$$\mu(x) = \sigma_{\min}(C), \quad C \equiv \begin{bmatrix} A & \frac{\|r\|}{\|x\|} \left( I - \frac{rr^T}{\|r\|^2} \right) \end{bmatrix}.$$

When  $m > n$  by a significant amount, it has been considered too expensive to evaluate  $\sigma_{\min}(C)$  directly. In a 2008 draft, Pete has shown that  $\mu(x)$  can be obtained much more cheaply from the smallest singular value of an  $(n + 1) \times 2n$  matrix derived from  $C$ . This is a computational breakthrough worthy of prompt publication.

Regrettably, Pete’s draft has been held up on my desk for a whole year, partly because many things happen from one line to the next, and because more symbols are needed than we actually have in the Roman and Greek alphabets. I’m always struggling to remember what  $Q_A$  and  $Q_{\perp}$  mean,<sup>1</sup> and I keep wanting to change many “we will”s into the present tense.<sup>2</sup> I am sure to lose both arguments, given Pete’s immense experience and astonishingly prolific contributions to the literature.

I mention this only to add that Pete is not *always* adamant! Long ago when he was inventing the name “downdating” for LINPACK’s  $\bar{R}^T \bar{R} \leftarrow R^T R - xx^T$  procedure (where  $x^T$  is a row of a matrix  $X$  for which  $X^T X = R^T R$ ), Pete wrote to ask for my thoughts about an algorithm he was proposing. I replied by letter from New Zealand that the method I had developed in my 1972 thesis [4] seemed to be rather simpler. Pete very graciously wrote back “Thank you for saving me from myself!” Ultimately, Pete implemented my simpler downdate and extended it to downdating the right-hand side and  $\|r\|$  of the associated least-squares problem. This has been called the LINPACK downdate ever since.

Even more impressively, Pete analyzed the downdating method and showed that it is stable (although  $\bar{R}$  can be a very ill-conditioned function of  $R$  and  $x$ ) [7]. Such error analyses have always been beyond me, so I have lived my life in awe of the few people like Pete who are able to do them.<sup>3</sup>

An intriguing aspect of the LINPACK downdate is that it solves  $R^T a = x$  and computes  $\alpha = \sqrt{1 - \|a\|^2}$ , which should be nonnegative if  $x^T$  really is a row of  $X$ . If  $\alpha \geq 0$ , the downdate will proceed without failure, but clearly there is scope for serious cancellation if  $\|a\|$  is close to 1. In my thesis,  $X$  was the transpose of the basis matrix in the simplex method for linear programming, and thus happened to be square. The downdate makes  $X$  rank-deficient by 1, but this was intentional because it’s the one time when we know the value of  $\alpha$  accurately:  $\alpha = 0$  *exactly*. (A subsequent *update* would restore the rank each simplex iteration.)

For many years I wished that someone like Pete would conduct an error analysis to confirm the imagined benefit of this  $\alpha = 0$  case. In the end it was Pete’s son, Michael Stewart, who resolved the question during a visit to Stanford. He showed that if row  $x^T$  has just been *added*, a downdate to delete it should be reliable, but if there are intervening downdates in which  $R$  is ill-conditioned, it probably will not work well [8].

Thus, may I close by noting that Pete Stewart’s contributions to our field, including his highly capable son, are far greater than any of us is likely to have appreciated. Warmest thanks Pete! (And more thanks to Michael!)

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<sup>1</sup>They’re from the QR factorization  $\begin{pmatrix} Q_A^* \\ Q_{\perp}^* \end{pmatrix} A = \begin{pmatrix} R \\ 0 \end{pmatrix}$ . I recommend  $A = (Y \ Z) \begin{pmatrix} R \\ 0 \end{pmatrix} = YR$ .

<sup>2</sup>I agree that the future tense is appropriate for text books and other educational writing, but for technical articles, “in section 4 we consider . . .” and “in the last section we establish . . .” seem importantly more direct.

<sup>3</sup>Pan [3] later gave a new error analysis and showed that the same downdate can be implemented with about half the operations. This feels like the last word on downdating!

## References

- [1] N. J. Higham. *Accuracy and Stability of Numerical Algorithms*. SIAM, Philadelphia, second edition, 2002.
- [2] C. C. Paige and M. A. Saunders. LSQR: An algorithm for sparse linear equations and sparse least squares. *ACM Transactions on Mathematical Software*, 8(1):43–71, 1982.
- [3] C.-T. Pan. A modification to the LINPACK downdating algorithm. *BIT*, 30:707–722, 1990.
- [4] M. A. Saunders. *Large-scale Linear Programming using the Cholesky Factorization*. PhD thesis, Stanford University, CA, 1972.
- [5] G. W. Stewart. An inverse perturbation theorem for the linear least squares problem. *SIGNUM Newsletter*, 10:39–40, 1975.
- [6] G. W. Stewart. Research, development and LINPACK. In J. R. Rice, editor, *Mathematical Software III*, pages 1–14. Academic Press, New York, 1977.
- [7] G. W. Stewart. The effects of rounding error on an algorithm for downdating a Cholesky factorization. *J. Inst. Math. Appl.*, 23:203–213, 1979.
- [8] Michael Stewart. The square downdating problem. Private communication, 1997.
- [9] B. Waldén, R. Karlson, and J.-G. Sun. Optimal backward perturbation bounds for the linear least squares problem. *Numerical Linear Algebra with Applications*, 2(3):271–286, 1995.