A CRITERION FOR TRUNCATION OF
THE QR-DECOMPOSITION ALGORITHM FOR
THE SINGULAR LINEAR LEAST
SQUARES PROBLEM

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Abstract.
A possible improvement of the Faddeev-Kublanovskaja-Faddeeva lower bound for the least singular value of \( R \) by using additional information about \( R \) is discussed. A fast algorithm is given for calculating such a bound using the diagonal elements and the elements of largest modulus in each row of \( R \).

1. Introduction.

The truncated QR-decomposition algorithm is an often used technique [1, 2] for the singular linear least squares problem:
Find the \( x \in \mathbb{R}^n \) with the smallest \( l_2 \) norm, \( \|x\|_2 \), that minimizes
\[
\|Ax - b\|_2
\]
where
\( A \) is \( m \times n \), \( \text{rank}(A) = k < n \) and \( b \in \mathbb{R}^m \).

One numerically stable algorithm for the QR-decomposition of \( A \) is the modified Gram-Schmidt orthogonalization [3] combined with column pivoting. With exact arithmetic, \( p \) steps of this algorithm will give the matrices \( Q_p, R_p \) and \( E_p \) in:
\[
AP = Q_pR_p + E_p
\]
where
\( Q_p \) is an \( m \times p \) matrix with orthonormal columns,
\( R_p \) is a \( p \times n \) matrix, upper triangular in the first \( p \) columns,
\( E_p \) is an \( m \times n \) matrix with the first \( p \) columns zero and the last \( n - p \) columns orthogonal to the columns of \( Q_p \),
and \( P \) is an \( n \times n \) permutation matrix.

In the sequel we assume that \( P \) is chosen so that for every \( p \), the last column of \( Q_{p+1} \) is parallel to the column with largest \( l_2 \) norm in

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This way of choosing P is referred to as the normalized column pivoting strategy.

Since \( \text{rank}(A) = k < n \) we have, with exact arithmetic, \( E_k = 0 \). The exact solution of (1.1) is then given by

\[
(1.3) \quad x = P^T(Q_kR_k)^+b
\]

where \( M^+ \) denotes the Moore-Penrose pseudoinverse of the matrix \( M \).

Wilkinson ([4], p. 160, 236) has shown that the effect of rounding errors can be introduced in the formula (1.2) by

\[
(1.4) \quad (A + G_p)P = Q_pR_p + E_p.
\]

\( R_p \) and essentially \( E_p \) are known from the computations, \( Q_p \) is the matrix in (1.2) and \( G_p \) can be bounded a priori

\[
(1.5) \quad \| G_p \|_E \leq \gamma 2^{-t} \| A \|_E.
\]

Here \( \gamma \) is a small constant which depends on details of the algorithm and the rounding process and \( t \) is the number of bits after the binary point in the computer word.

In practice, the rank of \( A \) may not be known in advance. In such cases it is sometimes appropriate to approximate \( A \) with a matrix of rank \( k_0 \) where \( k_0 \) is determined from

\[
(1.6) \quad \sigma_{k_0}(A) > \varepsilon \geq \sigma_{k_0+1}(A)
\]

where \( \varepsilon \) is a small positive number. (We assume the singular values to be ordered so that \( \sigma_i \leq \sigma_j, \, i > j \)). With this approach it is well known that "rank overestimation", i.e. choice of \( k_0 \) too large, will introduce a risk of obtaining a completely unreasonable solution [2]. Thus, strict but reasonably sharp lower bounds for \( \sigma_p(A), \, p=1,2,\ldots \) are required for a good choice of \( k_0 \) using (1.6). Such lower bounds can be obtained from

\[
(1.7) \quad \sigma_p(A) + \| G_p \|_E \geq \sigma_p(Q_pR_p + E_p) \geq \sigma_p(R_p).
\]

The last inequality is seen to hold by putting \( \sigma_p(Q_pR_p + E_p) = \sigma_p(R_p^TQ_p^T + E_p^T) \) and making the maximization in the Courant - Fischer theorem ([4], p. 101) in the orthogonal complement of the space spanned by the columns of \( E_p \). Unfortunately, calculation of \( \sigma_p(R_p), \, p=1,2,\ldots \) will require too much work to justify the use of \( QR \)-decomposition on (1.1) instead of complete singular value decomposition. In this situation, then, one would like to be able to give reasonably sharp lower bounds for \( \sigma_p(R_p) \) in each \( QR \)-step using the information available about \( R_p \) at a computational cost which is insignificant compared with that required for one \( QR \)-step.