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An Interval Analysis Approach to Rank Determination in Linear Least Squares Problems

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An Interval Analysis Approach to Rank
Determination in Linear Least Squares Problems
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The linear least squares problem $A \underline{x} \equiv \underline{b}$ has a unique solution only if the matrix A has full column rank. Numerical rank determination is difficult, especially in the presence of uncertainties in the elements of A . This paper proposes an interval analysis approach. We define a set of matrices A^I that contains all possible perturbations of A due to uncertainties and say that A^I is rank deficient if any member of A^I is rank deficient. A modification to the Q-R decomposition method of solution of the least squares problem allows a determination of the rank of A^I , and a partial interval analysis of the solution vector $\underline{x}$. This procedure requires the computation of R^{-1} . Another modification is proposed which determines the rank of A^I without computing R^{-1} . The additional computational effort is $O(N^2)$ where N is the column dimension of A .

1. Introduction

The linear least squares problem

$$(1.1) \quad A \underline{x} \approx \underline{b}$$

has a unique solution only if the matrix A is of full column rank. Numerical determination of rank is not always easy, especially in light of uncertainties in the elements of A . It is often the case that $A = (a_{ij})$ is known to be correct only within certain tolerances and the desired but unknown $\hat{A} = (\hat{a}_{ij})$ satisfies

$$(1.2) \quad \hat{a}_{ij} = a_{ij} + \psi_{ij}, \quad |\psi_{ij}| \leq \max(\gamma_{ij}|a_{ij}|, \delta_{ij})$$

where γ_{ij} , δ_{ij} are relative and absolute error bounds. The uncertainty in $\hat{A}$ may cause rather large uncertainties in the solution, $\underline{x}$. If any $\hat{A}$ in (1.2) is rank deficient, then a numerical solution may be completely incorrect.

It is essential that algorithms designed to solve linear least squares problems address the question of rank deficiency. A complete answer would require an extensive interval analysis and the arrays of bounds (γ_{ij}) and (δ_{ij}) (cf. Hanson and Smith, [7], [8]). For the most part this extra computation is unwarranted. In this paper we address the situation where the matrix is assumed to be of full rank. The most efficient algorithm for this case is the QR decomposition of A based upon Householder reflections (Golub [5]). We will show that a minor modification of this algorithm will yield bounds that help determine the rank of the numerically uncertain matrix A .

The algorithms proposed here yield as much information about the possible rank deficiency of A as a singular value decomposition (Golub and Kahan [4]). The computational cost of a singular value decomposition is difficult to predict because of the iterative part of the algorithm (cf. Lawson and Hanson, page 122). As a general rule, the total cost is 2 to 8 times that of the fixed part of the algorithm. The algorithms proposed here are less costly than even the fixed portion of the singular value decomposition.

1.1 Notation

We will use the following notation. Capital letters will denote matrices, underlined small letters will denote vectors, and small letters will denote scalars. The $M \times N$ ($M \geq N$) real valued matrix

$$A = (a_{ij}) = \begin{pmatrix} | & | & \cdots & | \\ \underline{a}_1 & \underline{a}_2 & \cdots & \underline{a}_N \\ | & | & \cdots & | \end{pmatrix}$$

has a singular value decomposition

$$A = U \Sigma V^*, \Sigma = \text{diag}(\sigma_1, \dots, \sigma_N), 0 \leq \sigma_N \leq \dots \leq \sigma_1,$$

where $U_{M \times N}$ and $V_{N \times N}$ are unitary matrices. We will use the vector norms

$$\|\underline{v}\|_{\infty} = \max_i |v_i|$$

$$\|\underline{v}\|_1 = \sum_i |v_i|$$

$$\|\underline{v}\|_2 = \left(\sum_i |v_i|^2 \right)^{1/2}$$

and matrix norms

$$\|A\|_{\infty} = \max_i \sum_j |a_{ij}|$$

$$\|A\|_1 = \max_j \sum_i |a_{ij}| = \max_j \|\underline{a}_j\|_1$$

$$\|A\|_2 = \max_{\|\underline{x}\|_2=1} \|A\underline{x}\|_2 = \sigma_1$$

$$\|A\|_F = \left(\sum_{i,j} (a_{ij})^2 \right)^{1/2} = \left(\sum_i \sigma_i^2 \right)^{1/2}.$$

The 2-norm may appear without subscript. The vector $\underline{e}_j$ will denote the j^{th} basis vector and $\underline{e} = (1, 1, \dots, 1)^T$. We will let

$$C_1(A) = \|A\|_1 \|A^+\|_1,$$

where A^+ is the pseudo-inverse of A , be the condition of A in the appropriate norm.

1.2 Problem Definition

Consider the set of matrices that includes all perturbations in (1.2). Let

$$(1.3) \quad A_0^I = \{A + \Psi : |\psi_{ij}| \leq \max(\gamma_{ij}|a_{ij}|, \delta_{ij})\}$$

We will say that A_0^I is of full rank if every $\hat{A} \in A_0^I$ is of full rank. A subset of columns of A_0^I will be said to be linearly independent if there exists no $\hat{A} \in A_0^I$ whose corresponding columns are linearly dependent. An independent set of interval columns will be said to be maximal if no larger independent set includes it. The $\text{Rank}(A_0^I)$ will be the index of the largest maximal independent set of columns of A_0^I . This yields

$$(1.4) \quad \text{Rank}(A_0^I) \leq \min_{A \in A_0^I} \text{Rank}(\hat{A})$$

Notice that $\{\underline{a}_1^I, \underline{a}_j^I\}$ and $\{\underline{a}_1^I, \underline{a}_k^I\}$ may both be dependent sets, while $\{\underline{a}_j^I, \underline{a}_k^I\}$ may be an independent set. In fact, one can construct matrices for which the inequality in (1.4) is strict. However, if the right hand side equals N , then equality holds.

A desirable result would be to find a largest maximal independent set of columns of A_0^I and produce an interval solution $\underline{x}^I$ that contains all possible solutions based upon this maximal set. Such a result is possible but requires an inordinate amount of computation and storage (cf. Moore [12], Hanson and Smith [7], [8]). The goal of this paper is to obtain as much of this information as possible at a moderate increase in computation and storage over the Businger-Golub QR algorithm (Businger and Golub [2]).

Consider a larger interval matrix in which the error bounds are the same throughout each column. Let

$$\gamma_j = \max_i |\gamma_{ij}|, \quad \delta_j = \max_i |\delta_{ij}|,$$

$$(1.5) \quad A_1^I = \{A + \Psi: |\psi_{ij}| \leq \max(\gamma_j |a_{ij}|, \delta_j)\}.$$

One can picture A_1^I as a matrix each of whose columns is represented by an M -dimensional box in R^M with sides parallel to the axes. The Householder reflections used in the QR decomposition rotate the vector about the origin. The sides of the box may no longer be parallel to the axes. For that reason we enclose the box in a ball. Let

$$(1.6) \quad \epsilon_j = \left(\sum_{i=1}^M \max(\gamma_j |a_{ij}|, \delta_j)^2 \right)^{1/2},$$

$$A_2^I = \{A + \Psi: \|\underline{\psi}_j\|_2 \leq \epsilon_j, j=1, \dots, N\}.$$

Finally, consider an interval definition based upon the Frobenius norm. Let

$$\epsilon = \left(\sum_{j=1}^N \epsilon_j^2 \right)^{1/2},$$

$$(1.7) \quad A_F^I = \{A + \Psi : \|\Psi\|_F \leq \epsilon\}.$$

This is the interval matrix underlying methods based upon singular values.

Notice that

$$(1.8) \quad A_0^I \subseteq A_1^I \subseteq A_2^I \subseteq A_F^I.$$

In this paper we will use A_2^I . It has that property that the set of perturbations is invariant to multiplication by a unitary matrix. While rank determination based upon A_2^I is not as precise as that based upon A_0^I , it is preferable to rank based upon A_F^I .

Suppose the matrix A has the QR factorization

$$(1.9) \quad A = QR,$$

where $R_{M \times N}$ is upper triangular and $Q_{M \times M}$ is unitary. If the column order of A is fixed so that the independent columns are ordered first, then the matrix R is unique up to multiplication from the left by a matrix $D = \text{diag}(\pm 1, \dots, \pm 1)$. Once R is fixed the first $K = \text{Rank}(A)$ columns of Q are unique, while the remaining $M-K$ columns span the null space of A^T . Let us define the interval matrix R^I to be the set of upper triangular matrices that result from a QR decomposition of matrices in A^I ; that is,

$$(1.10) \quad R_2^I = \{\hat{R} = R + \Omega : \hat{A} = \hat{Q}\hat{R}, \hat{A} \in A_2^I\}.$$

Notice that

$$(1.11) \quad \text{Rank}(R_2^I) = \text{Rank}(A_2^I).$$

Statements about the Rank (R_2^I) can be thought of as bounds on the size of the diagonal elements of the upper triangular perturbation matrices Ω .

1.3 Overview

We will show in Section 2 that while singular value decomposition yields a partial answer to the rank of A_2^I , an equally definitive answer can be garnered from a QR decomposition and inspection of quantities related to $\|R^{-1}\|_1$. The latter can be established with less computational effort. In Section 3 an algorithm will be proposed that embodies a nearly optimal row and column pivot strategy and determines a maximal set of independent columns of A_2^I . Further, a partial interval analysis of $\underline{x}^I$ will be presented. This algorithm requires the construction of R^{-1} as the QR decomposition proceeds but remains computationally more efficient than singular value decomposition. In Section 4 it will be shown that a maximal set of columns may be determined without constructing R^{-1} . The additional computation over the QR decomposition is $O(N^2)$. Section 5 will discuss numerical results.

This work is similar in nature to that of Golub, Klema, and Stewart [6]. There the goal is to find an acceptable reduced rank solution based upon A_F^I . Here we assume full rank and only consider reduced rank solutions when rank deficiency is detected. No comparison between reduced rank solutions is presented. Their algorithm requires more work and assumes less information about the uncertainties in A .

The bounds established in Section 4 are similar in nature to those of Cline, Moler, Stewart, and Wilkinson [3] and the $O(N)$ bounds of Anderson and Karasalo [1]. These papers deal with lower and upper

bounds of $C_1(R)$ respectively. The bounds of Section 4 also yield upper and lower bounds on $C_1(R)$. The lower bound is similar to that of Cline et al. and the upper bound will be better than that of Anderson and Karasalo. Moreover, upper and lower bounds are constructed for each column. These bounds are used to determine the independence of the columns. When the gap between the upper and lower bounds leaves independence in question, the exact value is computed.

This analysis precludes an accurate rank determination when a weighted least squares solution is sought in which the weights vary greatly in magnitude. Singular value analysis fails here as well. Further study is being conducted in an attempt to incorporate this case (cf. Powell and Reid [14]).

2. Rank of A_2^I

For convenience we will first assume that the columns of the matrix A have been scaled so that the uncertainty is the same in each. This does not affect the solution of (1.1). Later we will lift this restriction.

We have

$$(2.1) \quad A_2^I = \{A + \Psi : \|\Psi_j\|_2 < \epsilon, j = 1, \dots, N\},$$

$$(2.2) \quad R_2^I = \{\hat{R} : \hat{A} = \hat{Q} \hat{R}, \hat{A} \in A_2^I\}.$$

Let

$$(2.3) \quad \Psi_2^I = \{\Psi : \|\Psi_j\|_2 < \epsilon, j = 1, \dots, N\}.$$

2.1 Tests Based On Singular Values

We have the following well known result:

Theorem 2.1

If $\sigma_k < \epsilon$, then $\text{Rank } (A_2^I) < k$

If $\sigma_k > \epsilon \sqrt{N}$, then $\text{Rank } (A_2^I) > k$

Proof Notice that if $\Psi \in \Psi_2^I$, then $\|\Psi\|_F < \epsilon \sqrt{N}$. Further, notice that if $\|\Psi\|_F < \epsilon$, then $\Psi \in \Psi_2^I$. The theorem follows from well known results on singular values (cf. Stewart [13], page 320). ■

Thus, the singular values will determine the rank deficiency of A_2^I to within $\sqrt{N}$. In general, the $\sqrt{N}$ cannot be omitted.

2.2 Tests Based on R^{-1} .

Rank tests based upon $\|R^{-1}\|_1$ give similar results. First, let

$$(2.4) \quad R^{-1} = (\delta_{ij}), \quad \rho_j = \sum_{i=1}^j |\delta_{ij}|;$$

then,

$$(2.5) \quad \rho = \|R^{-1}\|_1 = \max_j \rho_j.$$

Theorem 2.2 Let $\{\rho_{j_\ell}\}_{\ell=1}^k$ be a subset of the ρ_j 's.

$$\text{If } \left(\sum_{\ell=1}^k \rho_{j_\ell}^2 \right)^{1/2} < \frac{1}{\epsilon}, \text{ then } \text{Rank } (A_2^I) > k.$$

Proof Let $A = QR$ be the QR decomposition of A . Assuming R is of full rank, then $\text{Rank } (A+\Psi) = \text{Rank } (I + Q^* \Psi R^{-1})$. If $k = N$, we have

$$\begin{aligned} \|\Psi R^{-1}\|_F &= \left(\sum_{j=1}^N \left(\sum_{i=1}^M \psi_i \delta_{ij} \right)^2 \right)^{1/2} \\ &< \left(\sum_{j=1}^N \left(\sum_{i=1}^M \|\psi_i\| |\delta_{ij}| \right)^2 \right)^{1/2} \\ &< \epsilon \left(\sum_{j=1}^N \rho_j^2 \right)^{1/2} < 1. \end{aligned}$$

If $k < N$, consider the submatrix of ΨR^{-1} consisting of those columns associated with the ρ_j 's in the subset. Denote this by

$(\Psi R^{-1})_k$. Again we have

$$\|(\Psi R^{-1})_k\|_F < 1,$$

which implies that these k columns are linearly independent for every

$\Psi \in \Psi_2^I$. The case in which R is singular is proved similarly. ■

The next result yields a more convenient form for rank determination.

Theorem 2.3

If $\rho > \frac{1}{\varepsilon}$, then A_2^I is rank deficient.

If $\rho < \frac{1}{\varepsilon\sqrt{N}}$, then A_2^I is of full rank.

Further, if $k = \text{index} \{ \rho_j : \rho_j < \frac{1}{\varepsilon\sqrt{N}} \}$, then $\text{Rank}(A_2^I) > k$.

Proof If $A = QR$ is the QR decomposition of A , then the matrix

$A = A + \Psi$, $\Psi \in \Psi_2^I$, has the same linearly independent sets of columns as the matrix $Q^*(A + \Psi) = R + \Phi$. Note that $\Phi \in \Psi^I$.

Assume $\rho_k > \frac{1}{\varepsilon}$ for some k . Define Ψ such that

$$\psi_i = -\text{sign}(\delta_{ik})/\rho_k \quad Q \quad e_k.$$

We have $\Psi \in \Psi_2^I$, and it is easy to show that

$$(R + \Phi)(R^{-1}e_k) \equiv 0.$$

Thus, A_2^I is rank deficient.

The last two results follow from Theorem 2.2. ■

This result is sharp in that the $\sqrt{N}$ cannot be omitted. Suppose A is such that $R^{-1} > 0$ and $\rho_j = \frac{1}{\varepsilon\sqrt{N}}$, $j = 1, \dots, N$. Then let Ψ be

such that $\psi_i = \frac{\varepsilon}{\sqrt{N}} Q e$, $(e = \sum_{i=1}^N e_i)$. We have $\Psi \in \Psi^I$, and

$$(R + Q\Psi)(R^{-1}e) = 0.$$

Thus, A is rank deficient. On the other hand, suppose

$$R^{-1} = \rho \begin{pmatrix} 1 & 1/2 & 1/3 \\ 0 & 1/2 & -1/3 \\ 0 & 0 & 1/3 \end{pmatrix}$$

One can show that for $\frac{1}{\epsilon\sqrt{N}} < \rho < \frac{3}{\epsilon\sqrt{22}}$ we have $\text{Rank}(A_2^I) = N$.

2.3 Implicit Scaling

Consider again the interval matrix (1.5) with perhaps different bounds for each column. A singular value analysis without first scaling the columns yields no information about A_2^I . This is not a major drawback in that column scaling so that the error is equal in each column is a standard practice. However, this scaling can be handled implicitly when bounds are based upon R^{-1} . As in (2.4), let

$$(2.6) \quad \rho_j = \sum_{i=1}^N |\delta_{ij}| \epsilon_i.$$

The following result is analogous to Theorem 2.3.

Theorem 2.4

If $\rho_j > 1$ for some j , then A_2^I is rank deficient.

If $\rho_j < \frac{1}{\sqrt{N}}$ for every j , then A_2^I is of full rank.

Further, if $k = \text{index} \{ \rho_j : \rho_j < \frac{1}{\sqrt{N}} \}$, then $\text{Rank}(A_2^I) > k$.

Proof Suppose $A \in A_2^I$. Let $E = \text{diag} \left(\frac{1}{\epsilon_1}, \dots, \frac{1}{\epsilon_N} \right)$; then,

$A E \in A_2^I$ with $\epsilon_j = \epsilon_j = 1$, $j = 1, \dots, N$. We can apply the results of Theorem 2.3 where we now substitute RE for R . Thus, we must find the $\|\cdot\|_1$ of the columns of $E^{-1}R^{-1}$. These are the quantities defined in (2.6). ■

2.4 Operation Count

A singular value decomposition involves an iteration and so it is difficult to accurately predict how much computational effort is

required. If the Golub algorithm is used (Golub [5]), the fixed computational effort is approximately $2MN^2$ floating point operations.¹ If a QR decomposition is followed by a singular value decomposition, the fixed computation is $MN^2 + 5N^3/6$ (Lawson and Hanson [10], page 122). The QR decomposition requires $MN^2 - N/3$ operations. Once R is known, the quantities ρ_j in (2.4) may be computed by successive back solves requiring $N^3/6$ operations and N words of storage. Thus, the QR algorithm with rank determination based upon $\|R^{-1}\|_1$ is computationally more efficient than singular value decomposition for determining the rank of A_2^I .

There are other advantages to computing R^{-1} . These will be discussed in Section 3. In Section 4 bounds will be developed that yield much of the same information with only $O(N^2)$ extra computation.

Section 3

In this section an algorithm will be presented which determines a maximal set of independent columns of A_2^I (up to a factor of $\sqrt{N}$). Also, bounds on the interval solution $\underline{x}^I$ based upon this maximal set are established.

Section 3.1 QR decomposition; row and column pivot strategy.

Consider the QR decomposition of A . Using the Golub algorithm (Golub [5]), the upper triangular matrix $R = A^{(N)}$ is computed in N steps where

$$A^{(k+1)} = H^{(k)} P_r^{(k)} A^{(k)} P_c^{(k)},$$

$P_r^{(k)}$, $P_c^{(k)}$ are row and column permutation matrices and $H^{(k)}$ is the Householder reflection matrix that zeros out the subdiagonal elements

1. Here, a floating point operation consists of one addition and one multiplication.

of the $k+1^{\text{st}}$ column of $P_r^{(k)} A^{(k)} P_c^{(k)}$. Suppose $\hat{A} = A + \Psi$, $\Psi \in \Psi_2^I$ is decomposed using the same row and column pivot order. We have

$$\hat{R} = R + \Omega$$

where Ω is also upper triangular. A consequence of the results in Manteuffel [11], (Section 4) and Theorem 2.2 yields the bound

$$(3.1) \quad |\omega_{kk}| < \left(\sum_{j=1}^k \rho_j^2 \right)^{1/2} |r_{kk}|, \quad k = 1, \dots, N,$$

where ω_{kk} is the k^{th} diagonal element of Ω and ρ_j is as in (2.6).

Also, from the proof of Theorem 2.3 we know that there exists a perturbation such that

$$|\omega_{kk}| > \rho_k |r_{kk}|.$$

The vector $\underline{\rho}$ provides bounds on the relative uncertainty of the diagonal elements of R . We would like to choose the column order so that the column with the smallest relative uncertainty comes first (cf. Manteuffel [11], page 31). Notice that if the uncertainty is the same in each column this corresponds to choosing the longest column as in the Businger-Golub algorithm [2]. The choice of the first column affects the size of the uncertainty in the truncated portion of the remaining columns. If one were to rescale at each step so that the truncated portion of the uncertainty were the same for each remaining column, then the algorithms presented here would be similar to that of Businger and Golub. We present an algorithm in which the columns are ordered so that ρ_k is as small as possible at step k . Also, a row pivot is used so that $H^{(k)}$ reflects onto the nearest basis element. This reduces the growth of the truncated portion of the uncertainty (cf. Manteuffel [11], page 31; Powell and Reid [14]).

3.2 Algorithm

Let us denote

$$(3.2) \quad A^{(k)} = \begin{pmatrix} R_{11}^{(k)} & R_{12}^{(k)} \\ 0 & R_{22}^{(k)} \end{pmatrix}$$

where $R_{11}^{(k)}$ is $k \times k$ and upper triangular. The elements of $R_{11}^{(k)}$ and $R_{12}^{(k)}$ are fixed (up to column interchanges in $R_{12}^{(k)}$) for step $k+1, \dots, N$.

We can construct the inverse of R as we proceed. Consider the matrix

$$(3.3) \quad \Delta^{(k)} = (\delta_{ij}^{(k)})$$

where the elements are updated at each step according to the formulas

$$(3.4) \quad \delta_{kk}^{(k)} = \frac{1}{r_{kk}};$$

for $i = 1, \dots, k-1$

$$(3.5) \quad \delta_{ik}^{(k)} = -\delta_{kk}^{(k)} \cdot \delta_{ik}^{(k-1)};$$

for $j = k+1, \dots, N$

for $i = 1, \dots, k-1$

$$(3.6) \quad \begin{aligned} \delta_{ij}^{(k)} &= \delta_{ij}^{(k-1)} + \delta_{ik}^{(k)} \cdot r_{kj}^{(k)}, \\ \delta_{kj}^{(k)} &= \delta_{kk}^{(k)} r_{kj}^{(k)} \end{aligned}$$

We may write

$$(3.7) \quad \Delta^{(k)} = \begin{pmatrix} \Delta_{11}^{(k)} & \Delta_{12}^{(k)} \\ 0 & \Delta_{22}^{(k)} \end{pmatrix},$$

where

$$(3.8) \quad \Delta_{11}^{(k)} = (R_{11}^{(k)})^{-1}, \quad \Delta_{12}^{(k)} = (R_{11}^{(k)})^{-1} R_{12}^{(k)}$$

and $\Delta_{22}^{(k)}$ is as yet undefined.

Clearly, after k steps we may compute the quantities ρ_j , $j=1, \dots, k$. Further, we may examine the columns of $\Delta_{12}^{(k)}$ to determine the column permutation that will yield the smallest ρ_{k+1} . Let $\underline{s}^{(k)}$ be the vector such that $s_j^{(k)}$ contains the $\|\cdot\|_2$ of the corresponding column of $R_{22}^{(k)}$. For $j = k+1, \dots, N$ let

$$(3.9) \quad \rho_j^{(k+1)} = \frac{1}{s_j^{(k)}} (\epsilon_{k+1} + \sum_{i=1}^k |\delta_{ij}^{(k)}| \epsilon_i).$$

If column j were to be chosen to be permuted to the $(k+1)^{\text{st}}$ position, the resulting ρ_{k+1} would be given by $\rho_j^{(k+1)}$. We then choose the column order so that

$$(3.10) \quad \rho_{k+1}^{(k+1)} < \rho_j^{(k+1)} \quad j = k+1, \dots, N.$$

(It should be noted that even though ρ_k is chosen to be as small as possible at each step, the inequality $\rho_k < \rho_{k+1}$ might not necessarily hold.)

Assume $\rho_j < \frac{1}{\sqrt{N}}$, $j < k$, and suppose $\rho_{k+1} = \rho_{k+1}^{(k+1)} < \frac{1}{\sqrt{N}}$. By Theorem 2.4 the interval columns $\{\underline{a}_1^I, \dots, \underline{a}_{k+1}^I\}$ are linearly independent and $\text{Rank}(\underline{A}_2^I) > k+1$. On the other hand, suppose that for some $j > k+1$ we have $\rho_j^{(k+1)} > 1$. By Theorem 2.4 we know that the interval columns $\{\underline{a}_1^I, \dots, \underline{a}_k^I, \underline{a}_j^I\}$ are dependent. Therefore, column j may not be used in computing a solution. This column should be ordered last and only the remaining columns need be considered.

Once the $(k+1)^{\text{st}}$ column has been chosen the rows are permuted so that the element with the largest absolute value in the first column of $R_{22}^{(k)}$ appears at the top of the column. The first column of $R_{22}^{(k)}$ will then be reflected onto the nearest basis element.

In this way a maximal set of independent columns will be constructed. The factor $\sqrt{N}$ that separates the tests for dependence and independence

may have to be dealt with. If N is not too large, then this factor may be insignificant. Further, since $A_0^I \subseteq A_2^I$ by proper inclusion we may feel safe in ignoring the $\sqrt{N}$. Suppose we construct a set of K_2 columns in this manner. We may then appeal to Theorem 2.2 and determine the largest set of columns, say K_1 columns, such that $\sum \rho_j^2 < 1$. We will then have

$$K_1 < \text{rank}(A_2^I) < K_2.$$

The gap between K_1 and K_2 will indicate how precise the rank determination is. Numerical results show that with few exceptions $K_1 = K_2$ (see Section 5).

The overall cost of this algorithm is MN^2 arithmetic operations. The QR decomposition requires $MN^2 - N^3/3$ operations, construction of Δ requires $N^3/6$ operations, and the selection of $\underline{\rho}$ requires $N^3/6$ operations. This is still less than the fixed number of operations required for a singular value decomposition, which is the smaller of $MN^2 + 5N^3/3$ or $2MN^2$. Note that Δ may be constructed over R so that the only extra storage needed is for the vector $\underline{\rho}$. The extra computation required to select the column pivot may be unwarranted. In Section 4 upper and lower bounds on ρ_k are constructed at a cost of $O(N^2)$ operations and the pivot strategy may be based upon these. In fact, these bounds do not require the construction of Δ . However, Δ may provide information about $\underline{x}^I$, the interval solution.

3.3 Bounds on Uncertainty

Once $\Delta = R^{-1}$ has been constructed both $\|R^{-1}\|_1$ and $\|R^{-1}\|_\infty$ may also be computed. The norms $\|R\|_1$ and $\|R\|_\infty$ can be computed during the decomposition. With these and the bound

$$C_2(A) \leq \sqrt{C_1(A)C_\infty(A)}$$

One can analyze the relative uncertainty in the various norms; that

is, the quantity

$$\frac{\|\underline{x} - \hat{\underline{x}}\|}{\|\underline{x}\|},$$

where $\hat{\underline{x}}$ is the solution of a perturbed system $\hat{A}\hat{\underline{x}} = \hat{\underline{b}}$, can be bounded (cf. Stewart [13], page 223).

We can also look at the term by term uncertainty to bound $\underline{x}^I$.

Let $\hat{A} = A + \Psi$, $\Psi \in \Psi_2^I$, $\hat{\underline{b}} = \underline{b} + \underline{\psi}_{N+1}$, $\|\underline{\psi}_{N+1}\|_2 \leq \epsilon_{N+1}$.

If we multiply both equations by Q we have

$$R\underline{x} = \underline{g}$$

$$(R + \Phi)\hat{\underline{x}} = \underline{g} + \underline{f}$$

where $\Phi \in \Psi_2^I$, $\|\underline{f}\|_2 \leq \epsilon_{N+1}$. We can write

$$(\underline{x} - \hat{\underline{x}}) = R^{-1}(\underline{f} - \Phi\hat{\underline{x}})$$

and

$$\begin{aligned} (3.12) \quad |\underline{x}_i - \hat{\underline{x}}_i| &= \left| \sum_k \delta_{ik} f_k - \sum_j \left(\sum_k \delta_{ik} \phi_{kj} \right) \hat{\underline{x}}_j \right| \\ &\leq \sum_k |\delta_{ik}| |f_k| + \sum_j \left(\sum_k |\delta_{ik}| |\phi_{kj}| \right) |\hat{\underline{x}}_j| \\ &\leq \|\underline{\delta}_i^T\|_2 (\epsilon_{N+1} + \sum_j \epsilon_j |\hat{\underline{x}}_j|) \end{aligned}$$

where $\underline{\delta}_i^T$ represents the i^{th} row of $\Delta = R^{-1}$. For small perturbations we may replace $|\hat{\underline{x}}_j|$ by $|\underline{x}_j|$ on the right hand side. This interval solution is fairly sharp in that we can always construct a perturbation such that

$$(3.13) \quad |\underline{x}_i - \hat{\underline{x}}_i| > \|\underline{\delta}_i^T\|_2 (\epsilon_{N+1} + \sum_j \epsilon_j |\hat{\underline{x}}_j|).$$

Of course (3.13) cannot be made to hold for all i simultaneously.

3.4 Reduced Rank Solutions

Suppose that A_2^I is found to be rank deficient and that a maximal set of $k < N$ independent columns has been established. Ignoring row and column pivoting, k steps of the standard QR algorithm would yield a system of the form

$$(3.14) \quad \begin{pmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{pmatrix} \begin{pmatrix} \underline{x}_1 \\ \underline{x}_2 \end{pmatrix} = \begin{pmatrix} \underline{g}_1 \\ \underline{g}_2 \end{pmatrix}$$

where R_{11} is $k \times k$ and upper triangular and $\underline{g} = Q^* \underline{b}$. The truncated least squares solution could be found by setting

$$\underline{x}_1 = R_{11}^{-1} \underline{g}_1$$

$$\underline{x}_2 = \underline{0}.$$

The minimal length least squares solution could be found by finding the minimal length solution to the undetermined system

$$(3.15) \quad \begin{pmatrix} R_{11} & R_{12} \end{pmatrix} \begin{pmatrix} \underline{x}_1 \\ \underline{x}_2 \end{pmatrix} = \underline{g}_1.$$

The algorithm of Section 3.2 produces the matrix

$$\Delta = \begin{pmatrix} \Delta_{11} & \Delta_{12} \\ 0 & R_{22} \end{pmatrix}$$

where $\Delta_{11} = R_{11}^{-1}$, $\Delta_{12} = R_{11}^{-1} R_{12}$. The truncated solution can be found using Δ by setting

$$\underline{x}_1 = \Delta_{11} \underline{g}_1$$

$$\underline{x}_2 = \underline{0}.$$

The minimal length least squares solution is more complicated.

Consider multiplying (3.15) by Δ_{11} . We have

$$(3.16) \quad \begin{pmatrix} I & \Delta_{12} \end{pmatrix} \begin{pmatrix} \underline{x}_1 \\ \underline{x}_2 \end{pmatrix} = \Delta_{11} \underline{g}_1.$$

The minimal length solution to (3.16) can be found by minimizing

$$\|\underline{x}_1\|_2^2 + \|\underline{x}_2\|_2^2 = \|\Delta_{11} \underline{g}_1 - \Delta_{12} \underline{x}_2\|_2^2 + \|\underline{x}_2\|_2^2.$$

This is equivalent to finding the solution to the least squares problem

$$(3.17) \quad \begin{pmatrix} \Delta_{12} \\ -I \end{pmatrix} \underline{x}_2 = \begin{pmatrix} \underline{f} \\ \underline{0} \end{pmatrix}$$

where $\underline{f} = \Delta_{11} \underline{g}_1$. The residual to (3.17) yields

$$(3.18) \quad \begin{pmatrix} \underline{x}_1 \\ \underline{x}_2 \end{pmatrix} = \begin{pmatrix} \underline{f} \\ 0 \end{pmatrix} - \begin{pmatrix} \Delta_{12} \\ -I \end{pmatrix} \underline{x}_2.$$

Suppose we construct an orthogonal matrix H as a product of Householder reflections such that

$$(3.19) \quad H \begin{pmatrix} \Delta_{12} \\ -I \end{pmatrix} = \begin{pmatrix} 0 \\ U \end{pmatrix}$$

where U is upper triangular. The residual of (3.17) is that

portion of $\begin{pmatrix} \underline{f} \\ 0 \end{pmatrix}$ that is orthogonal to $\begin{pmatrix} \Delta_{12} \\ -I \end{pmatrix}^T$ or H^* times that portion of $H \begin{pmatrix} \underline{f} \\ 0 \end{pmatrix}$ that is orthogonal to $\begin{pmatrix} 0 \\ U \end{pmatrix}^T$. We may write

$$(3.20) \quad \begin{pmatrix} \underline{x}_1 \\ \underline{x}_2 \end{pmatrix} = H^* \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} H \begin{pmatrix} \underline{f} \\ 0 \end{pmatrix}.$$

The transformation H can be constructed and stored over Δ_{12} and R_{22} . Notice that Δ_{11} remains intact so that both truncated solutions and minimal length solutions can be constructed for future right hand sides.

Section 4 $O(N^2)$ Bounds

In this section we develop an algorithm that determines a maximal linearly independent set of columns of A_2^I at an additional cost of $O(N^2)$ operations over the QR decomposition.

4.1 Upper and Lower Bounds

Let us again assume that the columns of A have been scaled so that $\epsilon = \epsilon_j$; $j = 1, \dots, N$. We will lift this restriction later.

Consider R to be an H -matrix³; then, the corresponding M -matrix² is

$$(4.1) \quad \bar{R} = (\bar{r}_{ij}); \quad \bar{r}_{ii} = |r_{ii}|; \quad \bar{r}_{ij} = -|r_{ij}|, \quad i \neq j.$$

Let us write

$$(4.2) \quad R = D(I-T), \quad D = \text{diag} (r_{11}, \dots, r_{NN}).$$

$$\bar{R} = \bar{D} (I - \bar{T}), \quad \bar{D} = \text{diag} (\bar{r}_{11}, \dots, \bar{r}_{NN}).$$

Then,

$$(4.3) \quad R^{-1} = (I + T + \dots + T^{N-1}) D^{-1},$$

$$\bar{R}^{-1} = (I + \bar{T} + \dots + \bar{T}^{N-1}) \bar{D}^{-1},$$

from which we see that

$$(4.4) \quad \bar{R}^{-1} > |R^{-1}| > 0.$$

If we denote $\bar{R}^{-1} = (\bar{\delta}_{ij})$, then

$$(4.5) \quad \bar{\rho}_j = \sum_{i=1}^j \bar{\delta}_{ij} > \sum_{i=1}^j |\delta_{ij}| = \rho_j.$$

Since $R^{-1} > 0$, the ρ_j 's can be computed with a single back solve. Let $\bar{\rho} = (\bar{\rho}_1, \dots, \bar{\rho}_N)^T$; then, if $\underline{e} = \sum_{i=1}^N \underline{e}_i$, we have

$$(4.6) \quad \bar{R}^{-T} \underline{e} = \bar{\rho}$$

and

$$(4.7) \quad \bar{\rho}_j = \frac{1}{|r_{jj}|} \left(1 + \sum_{i=1}^{j-1} |r_{ij}| \bar{\rho}_i \right).$$

The computation of $\bar{\rho}$ can be carried out during the QR decomposition and, in fact, $\bar{\rho}_k$ will be known after the k^{th} step of the QR algorithm.

Consider (4.6) with R^{-T} in place of $\bar{R}^{-T}$. If we let

$$(4.8) \quad R^{-T} \begin{pmatrix} \pm 1 \\ \cdot \\ \cdot \\ \cdot \\ \pm 1 \end{pmatrix} = \begin{pmatrix} \tilde{\rho}_1 \\ \cdot \\ \cdot \\ \cdot \\ \tilde{\rho}_N \end{pmatrix},$$

2. A matrix $A = (a_{ij})$ is an M-matrix, if $a_{ij} < 0$ for $i \neq j$, A is nonsingular and $A^{-1} > 0$.
3. A matrix $A = (a_{ij})$ is an H-matrix if the matrix $\bar{A} = (\bar{a}_{ij})$ with $\bar{a}_{ii} = |a_{ii}|$, $\bar{a}_{ij} = -|a_{ij}|$ $i \neq j$ is an M-matrix.

where the signs are to be chosen later, then we have

$$|\tilde{\rho}_j| = \left| \sum_{i=1}^j \pm \delta_{ij} \right| \leq \sum_{i=1}^j |\delta_{ij}| = \rho_j$$

Since R^T is lower triangular, we may write

$$(4.9) \quad R^T \tilde{\underline{\rho}} = \begin{pmatrix} \pm 1 \\ \vdots \\ \vdots \\ \pm 1 \end{pmatrix}$$

and choose the sign of the j^{th} element of the right hand side after $\tilde{\rho}_i$, $i < j$ have been computed. We may write

$$(4.10) \quad \tilde{\rho}_j = \frac{1}{r_{jj}} \left(\pm 1 - \sum_{i=1}^{j-1} r_{ij} \tilde{\rho}_i \right),$$

and choose the sign so that $|\tilde{\rho}_j|$ is as large as possible. Again, $\tilde{\rho}_k$ will be known after the k^{th} step of the QR decomposition. We have then

$$(4.11) \quad |\tilde{\rho}_j| \leq \rho_j \leq \bar{\rho}_j, \quad j = 1, \dots, N.$$

This yields the following corollary to Theorem 2.3.

Corollary 4.1

If $|\tilde{\rho}_j| > \frac{1}{\epsilon}$ for some j , then A_2^I is rank deficient.

If $\bar{\rho}_j < \frac{1}{\epsilon\sqrt{N}}$ for every j , then A_2^I is of full rank.

Further, if $k = \text{index} \{ \bar{\rho}_j : \bar{\rho}_j < \frac{1}{\epsilon\sqrt{N}} \}$, then $\text{Rank}(A^I) > k$.

The lower bounds $\tilde{\underline{\rho}}$ are computed in much the same manner as certain quantities in Cline, Moler, Stewart and Wilkinson ([3], page 371).

There they are concerned with what corresponds to $\|\underline{\rho}\|_2$ while here we are concerned with each individual $|\tilde{\rho}_j|$.

Following their development, we can enhance the lower bounds by looking ahead before choosing the sign. Suppose $\tilde{\rho}_j$, $j < k$ have

been chosen. Each $\tilde{\rho}_j$, $j > k$ is determined by

$$(4.12) \quad r_{jj}\tilde{\rho}_j = (-r_{1j}\tilde{\rho}_1 - \dots - r_{k-1j}\tilde{\rho}_{k-1}) + (-r_{kj}\tilde{\rho}_k - \dots - r_{j-1j}\tilde{\rho}_{j-1}^{\pm 1})$$

where the right hand side has been split into two parts. The first part is determined once $\tilde{\rho}_j$, $j < k$ have been chosen. Denote this part by $\tilde{\rho}_j^{(k-1)}$. The two values of ρ_k are

$$(4.13) \quad \tilde{\rho}_k = \frac{1}{r_{kk}}(\tilde{\rho}_k^{(k-1)} \pm 1)$$

We denote these by $\tilde{\rho}_k^+$ and $\tilde{\rho}_k^-$. We know that both values satisfy

$$(4.14) \quad |\tilde{\rho}_k^+| < \rho_k, \\ |\tilde{\rho}_k^-| < \rho_k,$$

and so may choose the larger in absolute value for our lower bound.

However, we are still free to choose either $\tilde{\rho}_k^+$ or $\tilde{\rho}_k^-$ for computation of $\rho_j^{(k)}$, $j > k$ as long as we are consistent throughout. Let

$$(4.15) \quad \tilde{\rho}_j^{(k)+} = \tilde{\rho}_j^{(k-1)} - r_{kj}\tilde{\rho}_k^+, \\ \tilde{\rho}_j^{(k)-} = \tilde{\rho}_j^{(k+1)} - r_{kj}\tilde{\rho}_k^+$$

and choose the sign to maximize

$$(4.16) \quad \sum_{j>k} |\tilde{\rho}_j^{(k)}|.$$

There is about twice as much work in this algorithm, but the overall work to compute $\tilde{\rho}$ remains $O(N^2)$. Notice that the

vector of bounds $\tilde{\underline{\rho}}$ does not necessarily satisfy (4.9) but will satisfy (4.11).

4.2 Implicit Scaling

As in Section (2.3) these bounds can incorporate implicit scaling. If we again consider A^I as in (1.5), then the formulas corresponding to (4.7) and (4.9) become

$$(4.15) \quad \bar{\rho}_j = \frac{1}{|r_{jj}|} (\epsilon_j + \sum_{i=1}^{j-1} |r_{ij}| \bar{\rho}_i),$$

$$(4.16) \quad \tilde{\rho}_j = \frac{1}{r_{jj}} (\pm \epsilon_j - \sum_{i=1}^{j-1} r_{ij} \tilde{\rho}_i).$$

This yields the following corollary to Theorem 2.4:

Corollary 4.2

If $|\tilde{\rho}_j| > 1$ for some j , then A_2^I is rank deficient.

If $\bar{\rho}_j < \frac{1}{\sqrt{N}}$ for every j , then A_2^I is of full rank.

Further, if $k = \text{index } \{\bar{\rho}_j: \bar{\rho}_j < \frac{1}{\sqrt{N}}\}$, then $\text{Rank}(A_2^I) > k$.

4.3 Construction of a Maximal Set

These bounds may be used in the pivot strategy and to construct a maximal set. Since $\rho_j < \bar{\rho}_j$ we have, as in (3.1), the bound

$$(4.17) \quad |\omega_{kk}| < \left(\sum_{j=1}^k \bar{\rho}_j^2 \right)^{1/2} |r_{kk}|, \quad k = 1, \dots, N.$$

Thus, we may choose the column order to make $\bar{\rho}_k$ as small as possible at each step. Suppose we compute $\bar{\underline{\rho}}^{(k)}$ as a vector of partial sums as we did for $\tilde{\underline{\rho}}^{(k)}$. Let

$$(4.18) \quad \rho_j^{(0)} = \epsilon_j, \quad j = 1, \dots, N$$

and at step k update $\bar{\underline{\rho}}^{(k)}$ by the formulas

$$(4.19) \quad \bar{\rho}_k^{(k)} = \frac{1}{r_{kk}} \bar{\rho}_k^{(k-1)} ;$$

for $j = k+1, \dots, N$

$$(4.20) \quad \bar{\rho}_j^{(k)} = \bar{\rho}_j^{(k-1)} + |r_{kj}| \bar{\rho}_k^{(k)}.$$

We have then $\bar{\rho}_k = \bar{\rho}_k^{(k)}$.

Again let $\underline{s}^{(k)}$ be the vector such that $s_j^{(k)}$ contains the $\|\cdot\|_2$ of the corresponding column of $R_{22}^{(k)}$. If column j were to be shifted to position $k+1$, then $\bar{\rho}_{k+1}$ would have the value $\frac{\bar{\rho}_j^{(k)}}{s_j^{(k)}}$. The pivot strategy is then to choose column $k+1$ so that

$$(4.21) \quad \bar{\rho}_{k+1} = \frac{\bar{\rho}_{k+1}^{(k)}}{s_{k+1}^{(k)}} < \frac{\bar{\rho}_j^{(k)}}{s_j^{(k)}}, \quad j = k+1, \dots, N,$$

Assume $\bar{\rho}_j < \frac{1}{\sqrt{N}}$, $j < k$, and suppose that $\bar{\rho}_{k+1} < \frac{1}{\sqrt{N}}$.

By Corollary 4.2 the interval columns $\{\underline{a}_1^I, \dots, \underline{a}_{k+1}^I\}$ are linearly independent and $\text{Rank}(A^I) > k+1$. On the other hand, suppose for some $j > k+1$ we have $|\tilde{\rho}_j| > 1$. By Corollary 4.2 we know that the interval columns $\{\underline{a}_1^I, \dots, \underline{a}_k^I, \underline{a}_j^I\}$ are linearly dependent and column j may not be used in computing a solution.

Suppose we have

$$(4.22) \quad \bar{\rho}_{k+1} > \frac{1}{\sqrt{N}}, \quad \tilde{\rho}_{k+1} < 1.$$

Corollary 4.2 yields no information. We must then compute the exact value ρ_{k+1} . This can be accomplished by a single back solve. Once ρ_{k+1} has been computed we may appeal to our previous strategy for determining linear dependence (see section

3.2). Since ρ_{k+1} is a better bound than $\bar{\rho}_{k+1}$ we may set $\bar{\rho}_{k+1}^{(k+1)} = \rho_{k+1}$ for computation of (4.20)

If A_2^I is assumed to be of full rank, that is, it is not clearly rank deficient from the outset, then the bounds $\bar{\rho}_k$ will most likely suffice for all but at most a few columns. In some of these columns $\tilde{\rho}_k$ may provide enough information. The exact value ρ_k will be computed $O(1)$ times for all but the most pathological problems. This yields an $O(N^2)$ algorithm that produces a maximal set of independent columns of A_2^I (up to the factor of $\sqrt{N}$).

5. Numerical Results

In this section we will compare the performance of the three algorithms described above: The algorithm of Section 3 that computes $R^{-1}(M1)$, the algorithm of Section 4 that creates upper and lower bounds (M2), and the algorithm of Section 4 that chooses the lower bound by looking ahead at partial sums (M3).

First, consider the following example that demonstrates the limitations of the Businger-Golub algorithm.

Let $s = \sin(\theta)$, $c = \cos(\theta)$,

$$A(\theta) = \begin{pmatrix} 1 & -c & -c & -c & \dots & -c \\ & s & -cs & -cs & \dots & -cs \\ & & s^2 & -cs^2 & \dots & -cs^2 \\ & & & s^3 & \dots & -cs^3 \\ & & & & \ddots & \\ & & & & & s^{N-1} \end{pmatrix}$$

For $0 < \theta < \frac{\pi}{2}$ the off diagonal terms remain negative. If we assume that the uncertainty is the same in each column; that is,

if we let

$$A_2^I = \{A + \Psi : \|\Psi\|_2 < \epsilon\},$$

then A_2^I is rank deficient for $\epsilon = (\frac{s}{1+c})^{N-1}$. To see this,

let $\Psi = -\epsilon \underline{e}_N \underline{e}^T$, and let

$$\underline{v} = \begin{pmatrix} c(1+c)^{N-2} \\ \vdots \\ \vdots \\ c(1+c) \\ c \\ 1 \end{pmatrix};$$

Then, we have

$$(A + \Psi) \underline{v} \equiv \underline{0}.$$

Both the Businger-Golub algorithm and the methods developed above would leave A unchanged. The Businger-Golub algorithm depends upon the size of the diagonal elements for rank determination.

With the proper choice of θ , ϵ can be made much smaller than s^{N-1} . For example, suppose we let $\epsilon = 10^{-13}$, $N = 53$, and $\theta = 58.70^\circ$. Then $s^{N-1} = 2.807 \times 10^{-4}$, but A_2^I is rank deficient.

To complicate matters $A(\pi-\theta)$, $0 < \theta < \frac{\pi}{2}$, has positive off diagonal elements and is quite well conditioned. The Businger-Golub algorithm is unable to differentiate between $A(\theta)$ and $A(\pi-\theta)$.

All three of the algorithms presented here properly detect the ranks of $A(\theta)$ and $A(\pi-\theta)$. The method M1 computes R^{-1} and so would be expected to correctly determine rank. For $A(\theta)$ both M2 and M3 compute exact bounds; that is, $\tilde{\rho} = \underline{\rho} = \overline{\rho}$. For $A(\pi-\theta)$, the lower and upper bounds are quite disparate: $\tilde{\rho} = \underline{\rho} \ll \overline{\rho}$. In the example cited above, however, only ρ_N needed to be computed exactly to determine the rank of A_2^I .

The ability of the three algorithms to determine numerical rank has been spelled out in the discussion above. However, several questions about their comparative performance must be answered by numerical tests.

Methods M2 and M3 will yield essentially the same pivot order, based upon the upper bounds $\bar{\rho}$. The difference between M2 and M3 lies in the computation of the lower bounds $\tilde{\rho}$. While M3 generally produces better bounds, the cost of computing those bounds is higher. The advantage to having better bounds lies in less frequent calculations of exact values of ρ . While M3 did compute fewer exact values, the difference was not sufficient to warrant the extra arithmetic as will be shown below.

In M1 the pivot order is determined by ρ , and so it may differ from the pivot order produced by M2, M3. While each algorithm will find a maximal set of independent columns, the numerical rank produced by M1 may differ from that produced by M2, M3. Even if the rank is the same, the maximal sets may contain different columns.

Four tests were performed. In each trial an $M \times N$ matrix $A = (a_{ij})$ was constructed with $N \in [10, 50]$, $M \in [N, 2N]$, and $a_{ij} \in [-1, 1]$ (each uniformly distributed). In the first test 2000 trials were run with relative uncertainty $\gamma_j = 10^{-4}$, $j = 1, \dots, N$ and absolute uncertainty $\delta_j = 10^{-4}$, $j = 1, \dots, N$. As might be expected, none of the trials produced a rank deficient matrix. Both M2 and M3 computed a total of 4 exact values of ρ . Figure 5.1 shows the distribution of $\frac{|\tilde{\rho}_j|}{\rho_j}$ and $\frac{\rho_j}{\bar{\rho}_j}$ for those trials in which M1 produced the same pivot order as M2, M3. The left half of Figure 5.1 shows the percent of the total with $\frac{|\tilde{\rho}_j|}{\rho_j} < x$ and the right half shows the percent of the total with $\frac{\rho_j}{\bar{\rho}_j} < x$.

In the second test 500 matrices were generated. Each matrix was given the four values $\gamma_j = \delta_j = 10^{-2}, 10^{-4}, 10^{-6}, 10^{-8}, j = 1, \dots, N$ for a total of 2000 trials. This test produced 1977 trials of full rank. Of the 23 rank deficient trials, M1 found the same maximal set as M2, M3 in 6 trials and the same rank in 19 trials. Method M2 computed 625 exact values of $\underline{\rho}$ while M3 computed 620. Figure 5.2 shows the distribution of $\frac{|\tilde{\rho}_j|}{\rho_j}$ and $\frac{\rho_j}{\rho_j}$ for those trials with identical pivot orders.

In the third test, after N and M were chosen, an integer K was chosen so that $N-K \leq 5$ and A was constructed so that the last N-K columns were linear combinations of the first K columns. Then a matrix $\Psi = (\psi_{ij})$ with $\psi_{ij} \in [-10^{-5}, 10^{-5}]$ was added to A. Each matrix was given the four values $\gamma_j = \delta_j = 10^{-2}, 10^{-4}, 10^{-6}, 10^{-8}, j = 1, \dots, N$ as in the second test. A total of 2000 trials were run. Only 896 trials were of full rank. Of the 1104 rank deficient trials, M1 found the same maximal set as M2, M3 in 951 trials and the same rank in 1078 trials. Method M2 computed 1495 exact values of $\underline{\rho}$ while M3 computed 1313. Figure 5.3 shows the distribution of $\frac{|\rho_j|}{\rho_j}$ and $\frac{\rho_j}{\rho_j}$ for those trials with identical pivot order.

In the fourth test A was chosen as in the first two tests, but relative and absolute uncertainties were chosen so that $\gamma_j = 10^{-NEX}, NEX \in [0, 14]$, and $\delta_j \in [0, 1]$ (uniformly distributed). Of 2000 trials only 101 were of full rank. Of the 1899 rank deficient trials M1 and M2, M3 found the same maximal set in 767 and the same rank in 1345. Method M2 computed 17,465 exact values of $\underline{\rho}$ while M3 computed 16,711. Figure 5.4 shows

Figure 5.1

Figure 5.2

Figure 5.3

Figure 5.4

the distribution of $\frac{|\tilde{\rho}_j|}{\rho_j}$ and $\frac{\rho_j}{\bar{\rho}_j}$ for those trials with identical pivot orders.

The first test is perhaps the most realistic set of problems. These algorithms were designed to handle problems that are assumed to be of full rank, with proper detection of that rare instance when rank deficiency occurs. Tests 2, 3, and 4 were constructed to produce increasingly more trials which are rank deficient and rank deficiencies of higher orders. In test 4 the absolute uncertainty is of the same magnitude as the elements of A.

We may conclude that there is enough similarity between the performance of algorithms M1 and M2, M3, in terms of finding a maximal set, that the extra computation required by M1 may be unwarranted. Method M1 does provide exact values for $C_1(R)$ and $C_\infty(R)$, but Figures 5.1 - 5.4 show that M2 and M3 also provide good bounds for $C_1(R)$. These bounds are best on the trials that are rank deficient or nearly rank deficient. Method M1 does provide bounds on $\underline{x}^I$ which cannot be extracted from M2 or M3.

The test results also show that M2 is more economical than M3. While Figures 5.1 - 5.4 show that M3 yields better lower bounds, more arithmetic was required to achieve the same results in terms of finding a maximal set.

In every trial in the first three test we had $K_1 = K_2$ so there was no doubt about the rank of A_2^I . In the fourth test there was uncertainty as to the rank in some trials but $K_2 - K_1$ never exceeded 3.

In addition, the length of the shortest least squares solution and the length of the residual vector produced by M1 were compared to

the corresponding values produced by the pseudo-inverse of the same rank. A singular value decomposition was used to construct the pseudo-inverse. As might be expected both pairs of values agreed to within the relative uncertainty used to compute the numerical rank with M1, sometimes many orders of magnitude less. This indicates that M1 is producing a good approximation to the pseudo-inverse.

Finally, M1 produced a column order in which $\rho_j < \rho_{j+1}$, $j=1, \dots, N-1$ in 95% of the 8000 trials.

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