

Stability of General Systems of Linear Equations

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To Professor Alexander Ostrowski, on his 75th birthday

1. Introduction

A common problem in many applications is to find minimal least squares to systems of simultaneous linear equations. By this we mean:

Given the $m \times n$ matrix A and the m -vector b , find an n -vector x which has minimum $\|Ax - b\|_2$ and that has minimum L_2 norm among all those vectors which have the same property.

It is well known that the solution to this problem is unique and given by

$$x = A^+ b$$

where A^+ is the Moore-Penrose pseudoinverse of A [8].

When the rank of A is well determined the computation of x as given does not constitute a very difficult problem and several working methods are [2, 4, 5, 7, 10].

When the rank of A is not well determined then the problem is ill-posed and standard methods fail to define an 'appropriate' solution. The term appropriate is casual since the violent ill-conditioning arising from almost linearly dependent columns of A makes it extremely difficult to define an x as in (1.1). This is due to the fact that small changes in the matrix A cause very large changes in the solution \hat{x} . See also [3, Chapt. 15] for an interesting discussion in this respect.

DEFINITION. Let A be an $m \times n$ matrix, b an m -vector, ε, δ two positive numbers. We shall say that A is ε, δ -stable with respect to b if for all matrix perturbations ΔA such that

$$\frac{\|\Delta A\|}{\|A\|} \leq \delta$$

the minimal least squares solutions $x = A^+ b, \hat{x} = (A + \Delta A)^+ b$ are such that

$$\frac{\|\hat{x} - x\|}{\|x\|} \leq \varepsilon.$$

A stronger concept than that of ε, δ -stability is the following:

Given the real non-negative number δ_0 , and the real non-negative function $\varepsilon(\delta)$ defined in $(0, \delta_0)$, we shall say that A is *strongly ε -stable at b* if the function

continuous at A and for any δ , $0 < \delta < \delta_0$

$$\|(A + \Delta A)^+ b - A^+ b\| \leq \varepsilon(\delta) \|A^+ b\|$$

provided that $\|\Delta A\| \leq \|A\| \delta$.¹⁾

Some properties of strong stability are:

(a) If A is strongly ε -stable then it is strongly ε' -stable for any ε' such that

$$\varepsilon(\delta) \leq \varepsilon'(\delta), \quad (0 < \delta < \delta_0).$$

(b) Because of the continuity there does exist an $\varepsilon(\delta)$ (in fact infinitely many) such that A is ε -stable and $\varepsilon(\delta) = o(1)$ as $\delta \rightarrow 0$.

(c) If A is strongly $\tilde{\varepsilon}$ -stable then it is ε , δ -stable for any ε such that $\tilde{\varepsilon}(\delta) \leq \varepsilon$.

Our intention is two-fold. On one side we shall find quantitative (and computable) a posteriori upper bounds for the relative variation

$$\frac{\|x - \tilde{x}\|}{\|x\|}$$

stemming from perturbations on the matrix A and the right hand side b . On the other side, we shall use these bounds in order to solve the following problem:

PROBLEM I. 'Given a general $m \times n$ matrix A , an m vector b , and ε , δ two positive numbers, find B , a set of linearly independent columns of A , such that $\tilde{A} = BB^+ A$ is ε , δ -stable with respect to b , and $\|(I - BB^+) A\| = \|A - \tilde{A}\|$ is minimum'.

This is another way of saying that, since the problem of finding minimal least squares solutions might be ill-conditioned, the user should supply the additional parameters ε , δ in order to make the problem well posed.

Observe that if B contains all the linearly independent columns of A then $\tilde{A} \equiv A$ and this will mean that A itself is ε , δ -stable and no modification of the given matrix is necessary in order to satisfy the requirements of the problem. Since the two conditions involved in Problem I are opposite, i.e. less columns will probably make \tilde{A} stable but will make the representation of A worse, it is clear that in this way we are trying to modify automatically the basic model A in order to make it stable, while simultaneously trying to introduce the minimum violence compatible with this purpose.

The method used in the analysis is non other than Wilkinson's 'backward error analysis' (see [13]).

The kinds of perturbations we allow are those that preserve the rank of A . In the course of the work we find a bound for

$$\frac{\|(E + \Delta E)^+ - E^+\|}{\|E^+\|}$$

¹⁾ The stability concepts introduced here are, of course, relative to the problem we are solving.

where E is a full rank matrix. Stewart [12] produces an L_2 bound of this general matrix A which does not seem to be comparable with ours. Ben obtains bounds for

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

in the case in which the equation $Ax=b$ is solvable (i.e. $b \in \text{range}(A)$), and perturbations ΔA are restricted not only in size but also to belong to a subspace which depends upon the matrix A . In this case he is able to obtain bounds which are better than the classical ones for nonsingular square matrices (cf. [3, 13]). Bjorck [15] and Wilkinson [14] also obtain bounds for the full rank case.

2. Notation and Definitions

The vector and matrix norms considered in this paper are any compatible norm. That is, norms satisfying

$$\|Ax\| \leq \|A\| \|x\|$$

for any matrix-vector pair for which the operation makes sense, and also the property $\|A\| = \|A^*\|$.²⁾

With regard to this last property we mention that if $\|\cdot\|$ is any matrix norm, then $\|A\| = \max(\|A\|, \|A^*\|)$ is a symmetric norm. In any case the use of this type of norm is not essential to obtain the results we are interested in, but makes the bookkeeping of intermediate computations simpler.

Some of the definitions below will be norm dependent. Unless it becomes necessary to clarify the context we will use but one symbol for the defined objects and we presume that a fixed norm is used throughout any given process.

DEFINITIONS. For a general $m \times n$ matrix A ($m \geq n$) we define:

- (a) A^+ the Moore-Penrose generalized inverse or pseudoinverse of A ; the unique $n \times m$ matrix which satisfies: (i) $AA^+A=A$, (ii) $A^+AA^+=A^+$, (iii) $(AA^+)^*=AA^+$, (iv) $(A^+A)^*=A^+A$ [8].
- (b) $\mathcal{R}(A) = \{y: y = Ax, x \in R_n\} \subset R_m$ the range subspace of A ;
- (c) $pk(A) = \|A^+\| \|A\| = pk(A^*)$ the pseudocondition number of A ;
- (d) $P_A = AA^+$ the orthogonal projection on the range subspace of A ;
- (e) $\hat{\angle} Ab$ the angle between a vector b and $\mathcal{R}(A)$;
- (f) We shall say that ΔA is a perturbation on A if the dimensions of the range of ΔA are equal to those of A and iff $\text{rank}(A + \Delta A) = \text{rank}(A)$.

²⁾ For any matrix A , A^* is the conjugate transpose or adjoint of A .

For an arbitrary matrix A and a perturbation ΔA we define the following functionals:

(g) $\omega(A) = pk(A) \frac{\|\Delta A\|}{\|A\|}$ the *amplified relative perturbation*;

(h) $\eta(A) = 1 + \omega(A)$;

(i) $\beta(A) = \omega(A) (\eta(A) + pk(A))$ the *regularity factor*;

(j) If $\frac{\|\Delta A\|}{\|A\|} \leq \delta$

$$\alpha(A) = \delta pk(A) [1 + pk(A) (\delta + 1)].$$

We recall some useful well known properties:

(k) A is a full column rank matrix iff A^*A is nonsingular. Furthermore we have in this case that

$$A^+ = (A^*A)^{-1}A^*;$$

(l) A is a full row rank matrix iff AA^* is nonsingular. Also

$$A^+ = A^*(AA^*)^{-1};$$

(m) If A is an arbitrary matrix and B is a subset of linearly independent columns of A that expand $\mathcal{R}(A)$ (i.e. B has full column rank = rank(A)) then

$$A = BC$$

where $C = B^+A$ has full row rank.

Proof. Assume that B is formed with the first columns of A , and call \bar{B} the matrix of the remaining columns; thus in block form we have $A = (B, \bar{B})$. Since the columns of \bar{B} are linearly dependent on the columns of B we can write $\bar{B} = B\tilde{B}$ for some matrix \tilde{B} . Thus

$$BB^+A = (BB^+B, BB^+B\tilde{B}) = (B, B\tilde{B}) = (B, \bar{B}) = A.$$

Also $C = B^+A = (I, \bar{B})$ since $B^+B = I$. Thus rank(C) = rank(A) = rank(B) = number of rows of C .

(n) $(A^+)^* = (A^*)^+$.

3. Perturbation of the Right Hand Side

We shall now study the effect that perturbations on the right hand side b have on the minimal least squares solution.

LEMMA 3.1. Let A be an $m \times n$ matrix, b and k m -vectors. Let $x = A^+b$. If $A \neq 0$ and b is not orthogonal to $\mathcal{R}(A)$ then the h that gives the minimal least squares solution

to $A(x+h)=b+k$ satisfies

$$\frac{\|h\|}{\|x\|} \leq pk(A) \frac{\|k\|}{\|P_A b\|}.$$

Proof. From its definition we obtain

$$h = A^+ k,$$

and therefore

$$\|h\| \leq \|A^+\| \|k\|.$$

On the other hand

$$Ax = AA^+ b = P_A b$$

and

$$\|P_A b\| \leq \|A\| \|x\|$$

which gives

$$\frac{\|P_A b\|}{\|A\|} \leq \|x\|.$$

Combining (3.2) and (3.3) we get

$$\frac{\|h\|}{\|x\|} \leq \|A\| \|A^+\| \frac{\|k\|}{\|P_A b\|},$$

which is (3.1).

Of course (3.2) is valid even if b is orthogonal to $\mathcal{R}(A)$, i.e. $AA^+ b=0$.

4. Continuity of $(\cdot)^+ b$. Full Rank Case

In this paragraph we shall prove that, for full rank matrices, $(\cdot)^+ b$ is continuous and moreover that those matrices are strongly ε -stable for suitable ε 's (and we shall exhibit).

First of all we produce a representation for the pseudoinverse of a perturbed rank matrix.

LEMMA 4.1. *Let E be a full rank matrix and ΔE a perturbation on it.*

$$\begin{aligned} \Omega &= E^+ \{ \Delta E + E^{*+} \Delta E^* (E + \Delta E) \}, \\ A &= \{ \Delta E + (E + \Delta E) \Delta E^* E^{*+} \} E^+. \end{aligned}$$

If E is full column rank then $(I + \Omega)$ is nonsingular and

$$(E + \Delta E)^+ = (I + \Omega)^{-1} E^+ (I + E^{*+} \Delta E^*).$$

If E is full row rank then $(I + A)$ is nonsingular and

$$(E + \Delta E)^+ = (I + \Delta E^* E^{*+}) E^+ (I + A)^{-1}.$$

Proof. Let E then be full column rank and let ΔE be a perturbation on E . Thus $(E + \Delta E)$ has full column rank (cf. § 2, (f)). Then $(E + \Delta E)^*(E + \Delta E)$ is nonsingular (cf. § 2, (k)), and we can write

$$\begin{aligned} (E + \Delta E)^*(E + \Delta E) &= E^*E + E^*\Delta E + \Delta E^*(E + \Delta E) \\ &= (E^*E) [I + E^+\Delta E + (E^*E)^{-1}\Delta E^*(E + \Delta E)] = (E^*E)(I + \Omega), \end{aligned} \tag{4.5}$$

where we used the identity $E^+E^{*+} = (E^*E)^{-1}E^*E(E^*E)^{-1} = (E^*E)^{-1}$.

Therefore $I + \Omega$ is nonsingular and

$$[(E + \Delta E)^*(E + \Delta E)]^{-1} = (I + \Omega)^{-1}(E^*E)^{-1}.$$

Finally

$$(E + \Delta E)^+ = (I + \Omega)^{-1}(E^*E)^{-1}(E^* + \Delta E^*) = (I + \Omega)^{-1}E^+(I + E^{*+}\Delta E^*)$$

which is (4.3).

Let E be a full row rank matrix and ΔE a perturbation on E . If we apply the first part of the Theorem to the full column rank matrix E^* and the corresponding perturbation ΔE^* , then by taking adjoints in the final result (4.4) follows. It is enough to observe that

$$\Lambda(E) = [\Omega(E^*)]^*. \tag{4.6}$$

LEMMA 4.2. *Let E be a full rank matrix and ΔE an arbitrary matrix of the same dimensions as E . If*

$$\beta(E) < 1 \tag{4.7}$$

then ΔE is a perturbation on E .

Proof. First of all, let E be a full column rank matrix. From (4.5) we deduce that $(E + \Delta E)$ has full column rank iff $(I + \Omega)$ is nonsingular. But $(I + \Omega)$ is nonsingular if $\|\Omega\| < 1$.

We shall show now that $\|\Omega\| \leq \beta(E)$ (thus the name of regularity factor we gave to $\beta(E)$).

$$\begin{aligned} \|\Omega\| &= \|E^+ \{ \Delta E + E^{*+} \Delta E^*(E + \Delta E) \}\| \\ &\leq \|E^+\| \|E\| \left\{ \frac{\|\Delta E\|}{\|E\|} + \|E^{*+}\| \|E^*\| \frac{\|\Delta E^*\|}{\|E^*\|} \left(1 + \frac{\|\Delta E\|}{\|E\|} \right) \right\} \\ &= \omega(E) (\eta(E) + pk(E)) = \beta(E). \end{aligned}$$

If E is of full row rank then a similar argument shows that for $(E + \Delta E)$ to be nonsingular it is sufficient that $\|\Lambda\| < 1$, and that also in this case $\|\Lambda\| \leq \beta(E)$. Therefore (4.7) implies, in both the full column and the full row rank cases, that $(E + \Delta E)$ is nonsingular and consequently that ΔE is a perturbation.

LEMMA 4.3. *Let $E, \Delta E$, and $\beta(E)$ be as in Lemma 4.2. Then*

$$\frac{\|(E + \Delta E)^+ b - E^+ b\|}{\|E^+ b\|} \leq \frac{1}{1 - \beta(E)} \left(\beta(E) + \omega(E) \frac{\|E^+\| \|b\|}{\|E^+ b\|} \right).$$

Proof. Again, we have to consider the full column and full row rank case rately. Let E be a full column rank matrix. According to (4.3) and using the Ne series for $(I + \Omega)^{-1}$ we get

$$(E + \Delta E)^+ b - E^+ b = \sum_{j=1}^{\infty} (-\Omega)^j E^+ b + \sum_{j=0}^{\infty} (-\Omega)^j E^+ E^{*+} \Delta E^* b$$

thus
$$\frac{\|(E + \Delta E)^+ b - E^+ b\|}{\|E^+ b\|} \leq \frac{1}{1 - \beta(E)} \left\{ \beta(E) + \|E^+\| pk(E) \frac{\|\Delta E\|}{\|E\|} \frac{\|b\|}{\|E^+ b\|} \right\}$$

A similar argument using the representation (4.4) gives the result for the f rank case.

COROLLARY 4.3. *Under the hypotheses of Lemma 4.3 we have that*

$$\frac{\|(E + \Delta E)^+ - E^+\|}{\|E^+\|} \leq \frac{\beta(E) + \omega(E)}{1 - \beta(E)}.$$

Now we can prove the main result of this Section.

THEOREM 4.4. *Let E be an $m \times n$ full rank matrix and b an m -vector non gonal to $\mathcal{R}(E)$. Let*

$$\begin{aligned} \delta_0(E) &= \frac{1}{2 pk(E)} \{ \sqrt{(1 + pk(E))^2 + 4} - (1 + pk(E)) \}, \\ \alpha(E) &= pk(E) \delta \{ 1 + pk(E) (\delta + 1) \}. \end{aligned}$$

For any $\delta < \delta_0$ let ΔE be any $m \times n$ matrix satisfying

$$\frac{\|\Delta E\|}{\|E\|} \leq \delta,$$

and let

$$\varepsilon(\delta) = \frac{1}{1 - \alpha} \{ \alpha + \delta pk(E)^2 \cos^{-1}(\widehat{Eb}) \}, \quad (0 < \delta < \delta_0). \quad ^3)$$

Then E is strongly ε -stable at b .

Proof. From (i) in §2 and (4.9) we see that for any $\delta < \delta_0$ and ΔE as speci corresponding $\beta(E) < 1$. Therefore Lemma 4.3 is applicable. Since

³⁾ Here $\cos^{-1}(Eb)$ is short hand for $\frac{\|b\|}{\|E^+ b\|}$. If the norm used is the Euclidean norm coincides with the standard trigonometrical notion.

$\|EE^+b\| \leq \|E\| \|E^+b\|$, then

$$\frac{\|EE^+b\|}{\|E\|} \leq \|E^+b\|$$

and from (4.8) we get that

$$\frac{\|(E + \Delta E)^+b - E^+b\|}{\|E^+b\|} \leq \frac{1}{1 - \beta(E)} \left\{ \beta(E) + pk(E)^2 \frac{\|\Delta E\|}{\|E\|} \cos^{-1}(\widehat{Eb}) \right\}, \tag{4.12}$$

or replacing

$$\frac{\|\Delta E\|}{\|E\|} \text{ by } \delta$$

$$\frac{\|(E + \Delta E)^+b - E^+b\|}{\|E^+b\|} \leq \frac{1}{1 - \alpha} \{ \alpha + \delta pk(E)^2 \cos^{-1}(\widehat{Eb}) \} = \varepsilon(\delta)$$

as we wanted to prove.

Observe that in the full row rank case $\cos^{-1}(\widehat{Eb})=1$.

5. The General Case

Let A be an arbitrary $m \times n$ matrix and ΔA a perturbation on it. Let B be a full rank matrix containing *all* the independent columns of A . Let $C=B^+A$; from (m) §2 we know that $A=BC$. Let ΔB be a matrix formed from ΔA by taking the same columns as those taken from A to form B . Let

$$\max \left(\frac{\|\Delta B\|}{\|B\|}, \frac{\|\Delta A\|}{\|A\|} \right) \leq \delta.$$

Let $\beta(B)<1$, so ΔB is a perturbation on B . Let ΔC be defined by means of the identity

$$C + \Delta C = (B + \Delta B)^+ (A + \Delta A). \tag{5.1}$$

(Observe that from the hypotheses it follows that $A + \Delta A = (B + \Delta B)(C + \Delta C)$.)

Now we want to find a bound for the relative perturbation

$$\frac{\|\Delta C\|}{\|C\|}.$$

LEMMA 5.1. *Let $A, B, C, \Delta A, \Delta B, \Delta C, \delta$ be as above. If $\alpha(B)<1$ then*

$$\frac{\|\Delta C\|}{\|C\|} \leq \frac{2\alpha(B)}{1 - \alpha(B)} \equiv \gamma. \tag{5.2}$$

Proof. $\Delta C = (B + \Delta B)^+(A + \Delta A) - C =$

$$[(I + \Omega)^{-1} - I] C + (I + \Omega)^{-1} B^+ [B^{*+} \Delta B^* (A + \Delta A) + \Delta A].$$

Thus

$$\frac{\|\Delta C\|}{\|C\|} \leq \frac{1}{1 - \beta(B)} \left\{ \beta(B) + \frac{\|B^+\| \|A\|}{\|C\|} (pk(B) \delta(1 + \delta) + \delta) \right\}.$$

Since $\beta(B) \leq \alpha(B)$ (5.2) follows.

We shall assume now that δ is so restricted as to ensure that $\beta(C) < 1$. Lemma 4.2 tells us that $C + \Delta C$ has full row rank. As we saw in Theorem 4, will be satisfied if

$$\frac{\|\Delta C\|}{\|C\|} \leq \gamma < \frac{1}{2pk(C)} \left\{ \sqrt{[1 + pk(C)]^2 + 4} - [1 + pk(C)] \right\} \equiv \delta'$$

We want to use the decomposition $A = BC$ (and $A + \Delta A = (B + \Delta B)(C + \Delta C)$ order to apply our results on the full rank case to this general problem. To do we proceed in two stages. Firstly we set the following least squares problem:

$$(B + \Delta B)(y + k) = b$$

where as usual $y = B^+b$.

Applying Theorem 4.4 to $B, \Delta B$ we see that

$$\frac{\|k\|}{\|y\|} \leq \frac{1}{1 - \alpha(B)} \left\{ \alpha(B) + \delta pk(B)^2 \cos^{-1}(\widehat{Bb}) \right\}.$$

Now we can set out a second least squares problem:

$$(C + \Delta C)(x + h) = y + k$$

where $x = C^+B^+b$, and this will give us the desired h . First we get

$$h = (C + \Delta C)^+(y + k) - C^+B^+b$$

and therefore

$$h = [(C + \Delta C)^+ - C^+]B^+b + (C + \Delta C)^+k.$$

Taking norms and dividing by $\|x\|$ we get

$$\frac{\|h\|}{\|x\|} \leq \frac{\|[(C + \Delta C)^+ - C^+]B^+b\|}{\|C^+B^+b\|} + \|C\| \|(C + \Delta C)^+\| \frac{\|k\|}{\|y\|},$$

where we have used the inequality

$$\frac{\|y\|}{\|C\|} \leq \|x\|,$$

which is easily obtained from $Cx = B^+b = y$. From (5.6) we now can prove the ineq result.

THEOREM 5.2. *Let A be an arbitrary $m \times n$ matrix, b an m -vector, B a maximal set of linearly independent columns of A , $C = B^+ A$. Let ΔA be an $m \times n$ matrix perturbation associated with A , ΔB the one corresponding to B as deduced from ΔA , and $\Delta C = (B + \Delta B)^+(A + \Delta A) - C$. If*

$$\max \left(\frac{\|\Delta A\|}{\|A\|}, \frac{\|\Delta B\|}{\|B\|} \right) \leq \delta$$

is so restricted as to make $\alpha(B) < 1$, and (5.3) is valid then A is ε -stable for

$$\varepsilon(\delta) = \frac{1}{1 - \alpha(C)} \left\{ \gamma pk(C)^2 + \alpha(C) + \frac{pk(C) \eta(C)}{1 - \alpha(B)} [\alpha(B) + \delta pk(B)^2 \cos^{-1}(\widehat{Bb})] \right\}. \tag{5.7}$$

Proof. The ε -stability of A , according to the def. in § 1 will be proved if for any perturbation ΔA on A , with norm less than $\delta \cdot \|A\|$, it follows that the h defined by $x + h = (A + \Delta A)^+ b$ ($x = A^+ b$) satisfies $\|h\| \leq \varepsilon(\delta) \|x\|$.

If in Theorem 4.4 we replace E by C and b by $B^+ b$ and then put the bound so obtained in (5.6) we get

$$\frac{\|h\|}{\|x\|} \leq \frac{1}{1 - \alpha(C)} (\alpha(C) + \gamma pk(C)^2) + \|C\| \|(C + \Delta C)^+\| \frac{\|k\|}{\|y\|}.$$

Using (5.5) and the representation for $(C + \Delta C)^+$ in this last expression we get

$$\begin{aligned} \frac{\|h\|}{\|x\|} &\leq \frac{1}{1 - \alpha(C)} (\alpha(C) + \gamma pk(C)^2) + \frac{\|C\| \|C^+\|}{1 - \alpha(C)} \eta(C) \\ &\times \frac{1}{1 - \alpha(B)} \{ \alpha(B) + \delta pk(B)^2 \cos^{-1}(\widehat{Bb}) \} = \varepsilon(\delta), \end{aligned}$$

as desired.

Observe that the whole expression is $O(\delta)$. The terms that are linear in δ and contain a factor of the form $pk(B)^2$ will be dominant in the case of ill conditioning. It is clear from its definition that C is well conditioned (all its singular values are 0 or 1), thus $pk(C)$ is not a troublesome quantity.

6. Applications

(a) *The Computation of Minimal Least Squares Solutions of Systems with Undetermined Rank*

We shall consider now how to apply the results of § 5 to the solution of Problem I (cf. § 1).

In [10] (see also [7, Chap. 2.4, §2a.1, pp. 369–372]) a method due to Rosen [11] for computing the pseudoinverse of a matrix was implemented as an Algol 60 program. Certain modifications introduced into the original procedure were implicitly directed

toward the solution of Problem I. The difficulty there was that the user had to provide some parameters which were, in principle, unrelated to the problem he wanted to solve, i.e. to find minimal least squares solutions. Well conditioned problems usual, did not create troubles. Our claim is that ill-posed problems of the form (1) are to be modified *before* any attempt is made to solve them. How to modify them depends, of course, on the user needs. What we propose in setting Problem I is in fact an automatic way of modifying ill designed models in order to eliminate highly correlated variables. The aim is to obtain answers which will behave smoothly with respect to the data, and to do that with minimum violence to the original model. The algorithm we propose now for solving Problem I can be implemented by introducing minor modifications to the computer program in [10].

Algorithm. A matrix B is constructed by considering the columns of A one by one. Recalling the statement of Problem I, let ε, δ be the stability parameters. We shall admit a column of A in the base B only if $\tilde{A} = BB^+A$ is ε, δ -stable. To implement this check, let us assume that B_q is a basis for which the corresponding \tilde{A}_q is ε, δ -stable and let u be a column of A , not in B_q , which is under examination. Let also $r_q = \|A - B_q B_q^+ A\|$. We shall provisionally form $B_{q+1} = (B_q, u)$, $C_{q+1} = B_{q+1}^+ A$, C_{q+1}^+ , and test $\tilde{A}_{q+1} = B_{q+1} C_{q+1}^+$ for ε, δ -stability according to (5.7). Of course it is assumed that u is *exactly* linearly dependent on the columns of B_q (in fact the limitation is overflowed by the computer in the computation of B_{q+1}^+), otherwise it is rejected a priori without further questioning.

If \tilde{A}_{q+1} is ε, δ -stable then we compute r_{q+1} and check if $r_{q+1} < r_q$; if so then u is accepted and B_{q+1} replaces B_q , otherwise u is rejected. If \tilde{A}_{q+1} does not satisfy condition (5.7) then u is also rejected.

In all cases, the next step is to examine the following column in A and so on until all the columns have been exhausted and a basis B satisfying the requirements of Problem I have been found.

Observe that the choice of a particular basis B depends upon the ordering of the columns of A (or rather, on the order in which they are taken for examination), that in any case only one cycle is necessary since a column which has been rejected when compared with a certain set of columns B' will certainly be rejected if compared with any set $B \supset B'$.

Let us call u a column of A that makes $\cos^{-1}(\widehat{bu})$ minimum. Assume for simplicity that $\|u\| = 1$. Then,

$$u^+ = \frac{\|u^*\|}{\|u\|^2} = 1,$$

and $pk(u) = 1$. Thus, a sufficient condition for Problem I to have a solution is

$$\delta \cdot \left[\frac{2 + \cos^{-1}(\widehat{bu}) + \delta}{1 - 2\delta - \delta^2} \right] \leq \varepsilon$$

where $\delta < \sqrt{2} - 1$; this is so because under those conditions $B \equiv u$ is ε , δ -stable (see Theorem 4.4).

(b) *Estimation of the Error Caused by a Model Modification.*

There are applications in which the dimensions of the matrix A are very large. In some cases the phenomenon under study allows one to modify A in such a way that the new model does not differ much from the original one but it has a simpler structure. For instance, in crystallographic computations it is known that in certain cases the normal equations of the linearized model are approximately block diagonal near the solution. What is more important, the size of the blocks is small compared to that of the original problem, where 200 parameters is not an unusual occurrence (cf. [9, specially paper 17, pp. 170–187 by R. A. Sparks] for more details).⁴

It is important in these cases to be able to estimate the effect of this modification on the computed least squares solution, and also the effect on the statistical quantities related to the elements of the inverse of the matrix of normal equations $A^T A$.

For this application the $m \times n$ matrix A will have full column rank and we shall then use the results of §4. Let then A and \tilde{A} be $m \times n$ full column rank matrices, $\Delta A = A - \tilde{A}$ be the perturbation, and b the right hand side vector. Let $x = A^+ b$, $\tilde{x} = \tilde{A}^+ b$. We want to estimate

$$\frac{\|h\|}{\|\tilde{x}\|} = \frac{\|x - \tilde{x}\|}{\|\tilde{x}\|}$$

in terms of

$$\frac{\|\Delta A\|}{\|\tilde{A}\|} \leq \delta, \quad pk(\tilde{A}),$$

and the other data of the problem. But this is exactly what we shall obtain from (4.12) in Theorem 4.4 if we put \tilde{A} instead of E and ΔA instead of ΔE . Recalling the definition of $\alpha(\tilde{A}) = pk(\tilde{A}) \delta [1 + pk(\tilde{A}) (\delta + 1)]$, and that $\beta(\tilde{A}) \leq \alpha(\tilde{A})$ we can write this result in the following way

$$\frac{\|x - \tilde{x}\|}{\|\tilde{x}\|} \leq \frac{\delta pk(\tilde{A})}{1 - \alpha(\tilde{A})} \{1 + pk(\tilde{A}) [\delta + \cos^{-1}(\widehat{\tilde{A}b}) + 1]\} \tag{6.1}$$

provided that $\alpha(\tilde{A}) < 1$.

From the decomposition (4.5) it follows that

$$\frac{\|(A^* A)^{-1} - (\tilde{A}^* \tilde{A})^{-1}\|}{\|(\tilde{A}^* \tilde{A})^{-1}\|} \leq \frac{\alpha(\tilde{A})}{1 - \alpha(\tilde{A})}. \tag{6.2}$$

The inequality (6.2) is nothing but a bound for the relative variation of the variance-covariance matrix for the derived parameters (cf. [6, Ch. 4]), due to the perturbation ΔA .

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