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A NUMERICAL METHOD OF DETECTING SINGULARITY OF A MATRIX

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16. Abstract The detection of matrix singularity by a numerical method is not easily accomplished on account of the finite precision of computer arithmetic.  In this paper we present a numerical method which determines a value $C$ for the degree of conditioning of a matrix. This value is $C = 0$ for a singular matrix and has progressively larger values for matrices which are increasingly well-conditioned. This value is $C = C_{\max}$ ( $C_{\max}$ defined by the precision of the computer) when the matrix is perfectly well conditioned.			
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# A NUMERICAL METHOD OF DETECTING SINGULARITY OF A MATRIX

M. La Porte and J. Vignes

## I. Introduction

/73\*

From a theoretical point of view, a matrix is singular if, and only if, the determinant of its coefficient is zero. Classical numerical algorithms permit calculating the value of a determinant. One such calculation carried out on a computer does not generally give a zero value for the determinant when the matrix is singular. In effect, the result obtained is vitiated due to the limited arithmetic precision of a computer. Then, there is always disagreement between the analytical result and the numerical result obtained on the computer. From this fact, it is apparent:

- a matrix, analytically non-singular, can appear as singular,
- a matrix, analytically singular, can appear as non-singular.

It is easy to give examples illustrating this disagreement. Let us consider the matrices:

$$A = \begin{bmatrix} 1 & 1 \\ 1+10^{-7} & 1 \end{bmatrix}, \quad A = \begin{bmatrix} 3 & 7 \\ 3 & 7 \end{bmatrix}.$$

The matrix  $A$  is regular and its determinant has a value of  $10^{-7}$ . The  $B$  matrix is singular.

Let us treat these two matrices on an imaginary computer operating to 7 significant points, arithmetically at a normalized floating comma with truncation.

The matrix  $A$  is presented in the form:

$$A = [A_{ij}]$$

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\*Numbers in the margin indicate pagination in the foreign text.

all of the  $A_{ij}$  being equal to 1. Then one has  $A \neq A$ . The value  $\Delta_A$  of determinant  $A$ , calculated with any algorithm, is zero. This matrix appears then as singular when it is not analytically.

The  $B$  matrix is presented in the form  $B = B$  since its coefficients fall correctly in the machine. Its determinant, calculated using a Gaussian algorithm with study of the maximal center-point by column, has a value of:

$$\Delta_B = 3 \times 10^{-9}$$

Then, this matrix appears as non-singular when it is obviously singular.

These two examples show the difficulty in detection, by an exclusively numerical method, of the singularity of one matrix.

These studies bearing on the propagation of numerical errors during calculation and their incidence in linear algebra have been made particularly by: Forsythe [1], Gastinel [2], Golub [3], Householder [4, 5], Wilkinson [7-10].

## II. Definition of Numerical Singularity

If the calculation of a determinant of an analytical singular matrix has a value which is not zero, one can confirm that this value is only the result of a cumulative effect of errors caused by the arithmetic of the computer. From this fact, this value is not significant and, consequently, it must be considered as mathematically zero.

Moreover, if the calculation of the determinant of an analytically non-singular matrix gives a zero value, one can say that on this computer this matrix appears as singular whereas it does not analytically. This necessitates going beyond the concept of analytical singularity in order to arrive at the concept of numerical singularity; for this we propose the following

definition:

Definition. A matrix is numerically singular when the value of its determinant, calculated on the computer, is:

- either zero,
- or not significant.

Let us consider a matrix  $A$  in which the coefficients  $a_{ij}$  are the algebraic values:

$$\mathcal{A} = [a_{ij}]. \quad (1)$$

Let us designate as  $A$  the image on the machine  $A$  and by  $A_{ij}$  the images of  $a_{ij}$ . In general, the  $A_{ij}$  are not strictly equal to  $a_{ij}$  due to error engendered by the periodic block operator [1, 5, 6].

They may be:

- $\text{Det}(A)$  the algebraic value of the determinant of  $A$ ,
- $\Delta_1$  the value calculated on the computer of determinant  $A$ ,
- $\epsilon$  the absolute error committed on  $\Delta_1$

$$\epsilon = \Delta_1 - \text{Det}(\mathcal{A}). \quad (2)$$

If the error  $\epsilon$  is of the same order of magnitude as the value  $\Delta_1$ , one can confirm that this latter is not significant. Consequently, the matrix must be considered as numerically singular.

If  $\epsilon$  is smaller than  $\Delta_1$ , then the matrix is not singular. /75

It is impossible to calculate  $\epsilon$  by (2) since the value of  $\text{Det}(A)$  is unattainable. Here we will present a method which, by statistical methods, makes it possible to estimate  $\epsilon$ .

### III. Origins of Error

Absolute error  $\epsilon$ , given by equality (2), has two distinct origins.

a) error in calculation. This corresponds to the cumulative effect of errors caused by each of the elementary operations carried out on the computer during calculation of  $\Delta_1$ : [1, 6, 7].

b) error in the coefficients. The coefficients  $A_{ij}$  of matrix  $A$  are not in general equal to the coefficient  $a_{ij}$  of the algebraic matrix  $A$  since they depend on part of the operator periodic block, and the other part on the origin of  $a_{ij}$ . Three cases can be presented:

Case 1. The  $a_{ij}$  are known exactly and go correctly into the machine. In this case:  $A = A$ .

Case 2. The  $a_{ij}$  are known exactly but do not fall correctly in the machine.  $A$  is an approximation of  $A$ , the error on the coefficient  $A_{ij}$  proceed only from a single operator periodic block.

Case 3. The  $a_{ij}$  are known with a certain error; this is the case, for example, when the  $a_{ij}$  result from experimental measurement. In this case, the periodic block error is negligible and the  $A_{ij}$  are affected by the same error as the  $a_{ij}$ .

We are going to determine, by a statistical method, a mean estimate of error  $\epsilon$ , starting with the populations created differently following the origin of error. The elements of these populations are the different numerical values of the the same determinant.

--if the  $a_{ij}$  correspond in the first case, only error in calculation has to be considered and the corresponding population is obtained by a "permutation" method.

--if the  $a_{ij}$  correspond to the second and third cases, the error in the coefficients and the error in the computation must be taken into account and the corresponding populations obtained by a "permutation-perturbation" method.

#### IV. Permutation Method (Theoretical Aspect)

This method applies to the first case, that is to say, when the coefficients  $A_{ij}$  of  $A$  are the exact image of coefficients  $a_{ij}$  and  $A$ .

$$A_{ij} = a_{ij}. \quad (3)$$

During calculation on a computer of the value of  $\Delta_1$ , the absolute error committed  $\epsilon$  is uniquely caused by the limited arithmetic precision of the machine. Due to this, it depends on the order in which the operations are carried out.

Also, in permuting the columns of  $A$ , one changes the order of operations and if one calculates the determinant, one obtains different value of  $\Delta_1$ .

By making all of the possible permutations of the column of matrix  $A$  in  $n$  order, one obtains  $n!$  matrices. Machine computation of  $n!$  corresponding determinants produces a population  $D_1$ . /76

$$D_1 = \{\Delta_1, \Delta_2, \dots, \Delta_n, \dots\}.$$

All of the values of  $\Delta_1$  are also represented by one or another value of  $\text{Det}(A)$ .

Also, the permutation method makes it possible to theoretically obtain a population  $D_1$  of the cardinal:

$$\text{Card } D_1 = n! \quad (4)$$

## V. Permutation-perturbation Method (Theoretical Aspect)

This method is applied to the second and third cases, that is to say, when the coefficients  $a_{ij}$  do not fall correctly in the machine. Then one has:

$$A_{ij} = a_{ij}(1 + \lambda_{ij}). \quad (5)$$

When one is in case No. 2, the  $\lambda_{ij}$  correspond to periodic block error and belong to the  $P(\alpha)$  population defined in [6] § 2.2. Then, one has:

$$A_{ij} = a_{ij}(1 + \alpha_{ij}) \quad \alpha_{ij} \in P(\alpha). \quad (6)$$

When one is in case No. 3, the  $\lambda_{ij}$  correspond to those experimental errors in which one assumes a higher boundary  $e_{ij}$  as known. Then, one has:

$$A_{ij} \in [a_{ij}(1 - e_{ij}), a_{ij}(1 + e_{ij})]. \quad (7)$$

In the case defined by (6), only two representations on the computer exist for each of the values of  $a_{ij}$ , the one by efficiency,  $A_{ij}^-$ , the other by excess  $A_{ij}^+$  and one has:

$$a_{ij} \in [A_{ij}^-, A_{ij}^+]. \quad (8)$$

If one works out all of the resulting matrices from a combination of the two possible states of each of the coefficients, one obtains  $2^{n^1}$  matrices. By applying the permutation method to each of these matrices, one obtains a population  $D_2$ :

$$D_2 = \{A_1, A_2, \dots, A_n, \dots\} \quad (9)$$
$$\text{Card } D_2 = n! 2^{n^1}.$$

In the case defined by (7), for each of the  $a_{ij}$ , there exist  $p_{ij}$  representations on the computer.

If one works out all of the matrices resulting from a combination of  $p_{ij}$  possible states from each of the coefficients, one obtains  $N$  matrices:

$$N = \prod_{i=1}^n \prod_{j=1}^n p_{ij} \quad (10)$$

In applying the computation method to each of these matrices, one obtains a population  $D_3$ :

$$D_3 = \{\Delta_1, \Delta_2, \dots, \Delta_N, \dots\} \quad (11)$$

$$\text{Card } D_3 = n! \prod_{i=1}^n \prod_{j=1}^n p_{ij}$$

## VI. Evaluation of $\hat{\epsilon}$ (Theoretical Aspect)

/77

Using the elements  $\Delta_i$  of one of the populations we find above:

$$D = \{\Delta_1, \Delta_2, \dots, \Delta_N\} \quad (12)$$

we will get a mean estimate of  $\hat{\epsilon}$  of absolute error  $\epsilon$  defined by:

$$\epsilon = \Delta_1 - \text{Det}(A) \quad (13)$$

with  $\Delta_1$  = the cacluated value on the computer of determinant  $A$   
 $\text{Det}(A)$  = the exact value of the determinant of  $A$ .

Here we can make the following hypothesis:

Hypothesis. During calculation of  $\Delta_1$  on the computer, the calculation errors of data have behaved indifferently in one direction or the other. Consequently, the value of  $\text{Det}(A)$  can be considered as an element of any of the  $D$  population.

We will call  $\bar{\Delta}$  and  $\delta^2$ , respectively, the mean and the variants of this population. Under the preceding hypothesis, the mean of error square  $\epsilon$  is expressed by:

$$\bar{\epsilon}^2 = (\Delta_1 - \bar{\Delta})^2 + \delta^2. \quad (14)$$

By definition, we suppose:

$$\bar{\epsilon}^2 = \epsilon^2 \quad (15)$$

or

$$\bar{\epsilon} = \sqrt{(\Delta_1 - \bar{\Delta})^2 + \delta^2}. \quad (16)$$

The value of  $\bar{\epsilon}$  compared to that of  $\Delta_1$  gives us information on the conditioning of the matrix. In the measurement where  $\Delta_1$  and  $\bar{\epsilon}$  are not zero, one can always write:

$$\frac{\bar{\epsilon}}{|\Delta_1|} = 10^{-C} \quad (17)$$

C represents the exact number of significant figures of  $\Delta_1$ . Of course, the value of C can never exceed the number  $C_{\max}$  of significant decimals in the arithmetic of the computer. If p designates the number of bits of the mantissa representing a normalized floating binary comma,  $C_{\max}$  is defined by:

$$2^p = 10^{C_{\max}}. \quad (18)$$

Then, three cases can be considered:

--C is in the neighborhood of  $C_{\max}$ : the matrix is numerically well conditioned.

--C is in the neighborhood of zero: the matrix is numerically singular.

--Between the two extreme cases, the matrix without being singular is not numerically well conditioned.

We will say that the matrix is numerically singular if the value of its determinant is known with less than an exact significant figure, that is to say, if  $C < 1$ .

## VII. Practical Aspect of the Permutation and Perturbation Methods

In practice, it is impossible to work out the totality of the population elements previously defined. We propose an algorithm which, with a number of limitations, makes it possible nevertheless to determine the number  $C$ .

Using any algorithm from calculation of the determinant, one defines the value of  $\Delta_1$  from the determinant of matrix  $A$  and the value of  $\Delta_2$  of the determinant of the matrix deduced from  $A$  by central symmetry. The interesting thing about this choice is the fact that during calculation of  $\Delta_1$  and  $\Delta_2$ , the errors are propagated in a very different way.

/78

Using these two elements, one calculates by (17) the value of  $C$ :

--if  $C < 1$ , then the matrix is numerically singular,

--if  $C \geq 1$ , the algorithm must be pursued by creating new elements of the  $D$  population until one obtains a stationary condition for the entire part of  $C$ . The successive elements of  $D$  are obtained by random permutation of the columns of matrix  $A$  and, should the occasion arise, by random perturbation of the  $A_{ij}$  coefficients. This perturbation consists of:

--in case No. 2, by random adjustment of a zero or a 1 at the last bit of the mantissa,

--in case No. 3, by replacing  $A_{ij}$  by:

$$A_{ij, \text{perturbed}} = A_{ij}(1 + \theta_{ij}e_{ij}) \quad (19)$$

$\theta_{ij}$  randomly takes the value -1 or +1.

### VIII. Agreement Between Theory and Practice

The permutation-perturbation method has been applied to a very large number of matrices of all orders and all conditions. This method has never been deficient. We will content ourselves with giving three important examples here.

#### VIII-1. Application of the Hilbert Matrix

The Hilbert matrix is a symmetrical matrix in which the terms are the inverse of successive integrals.

$$\mathcal{H}_n = \begin{bmatrix} 1 & 1/2 & 1/3 & \dots & 1/n \\ 1/2 & 1/3 & 1/4 & \dots & 1/(n+1) \\ 1/3 & 1/4 & 1/5 & \dots & 1/(n+2) \\ \dots & \dots & \dots & \dots & \dots \\ 1/n & 1/(n+1) & 1/(n+2) & \dots & 1/(2n-1) \end{bmatrix}$$

Using the Gaussian algorithm, one calculated on a CDC 7600 computer for  $n$  variants of 2 to 13, the value of  $\Delta_1$  then the value of  $C$  by the permutation and perturbation method (case No. 2).

Likewise, one knows the algebraic expression of the determinant of  $A_n$ :

with

$$\text{Det}(\mathcal{H}_n) = \frac{\psi^4(n-1)}{\psi(2n-1)}$$
$$\psi(n) = \prod_{i=0}^{i=n} (i!).$$

(20)

one can deduce from this the exact value of  $C$ , or  $C^*$ , defined by:

$$\left| \frac{\text{Det}(\mathcal{H}_n) - \Delta_1}{\text{Det}(\mathcal{H}_n)} \right| = 10^{-C^*}.$$

(21)

The results presented in Table I show that:

--on the one hand, perfect agreement between theory and practice (with values of C and C\* are similar),

--on the other hand, the small number of calculations of determinants  $\Delta_i$  necessary for obtaining the results.

Table I

n	Det( $\mathcal{M}_n$ )	$\Delta_i$	Number of $\Delta_i$ calculations	Either part		$S^*$
				C	C*	
2	$8.3 \times 10^{-2}$	$8.3 \times 10^{-2}$	4	13	14	
3	$4.6 \times 10^{-4}$	$4.6 \times 10^{-4}$	3	12	12	
4	$1.6 \times 10^{-7}$	$1.6 \times 10^{-7}$	3	11	10	
5	$3.7 \times 10^{-13}$	$3.7 \times 10^{-13}$	3	9	9	
6	$5.3 \times 10^{-18}$	$5.3 \times 10^{-18}$	3	8	8	
7	$4.8 \times 10^{-23}$	$4.8 \times 10^{-23}$	4	7	7	
8	$2.7 \times 10^{-28}$	$2.7 \times 10^{-28}$	4	5	6	
9	$9.7 \times 10^{-33}$	$9.7 \times 10^{-33}$	3	4	4	
10	$2.1 \times 10^{-38}$	$2.1 \times 10^{-38}$	3	3	2	
11	$3.0 \times 10^{-43}$	$2.3 \times 10^{-43}$	3	1	1	
12	$2.6 \times 10^{-48}$	$-4.5 \times 10^{-48}$	2	0	0	S
13	$1.4 \times 10^{-53}$	$-7.8 \times 10^{-53}$	3	0	0	S

S: numerically singular matrix.

VIII-2. Application of Least Squares to a Matrix

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Let us consider the matrix

$$\mathcal{M}_{N,p} = \begin{bmatrix} S_{1p} & S_{1p-1} & \dots & S_p \\ S_{2p} & S_{2p-1} & \dots & S_{p-1} \\ \vdots & \vdots & \dots & \vdots \\ S_p & S_{p-1} & \dots & S_0 \end{bmatrix} \text{ with } S_h = \sum_{i=0}^{i=N} i^h$$

which one encounters in certain polynomial adjustments by least squares.

The results obtained for N = 20 and p variations of 1 to 12 /80 are presented in Table II. This shows the good agreement between C and C\* and also shows that a matrix can be numerically singular itself if the order of magnitude of its determinant is very high.

Table II

$p$	$\text{Det}(A_{20,p})$	$A_1$	Number of $A_1$ calculations	Either part C of C*	S*
1	$1.6 \times 10^1$	$1.6 \times 10^1$	3	13	13
2	$3.6 \times 10^2$	$3.6 \times 10^2$	4	12	12
3	$2.2 \times 10^3$	$2.2 \times 10^3$	4	11	11
4	$3.8 \times 10^4$	$3.8 \times 10^4$	3	10	10
5	$1.7 \times 10^5$	$1.7 \times 10^5$	3	8	8
6	$1.9 \times 10^6$	$1.9 \times 10^6$	3	7	7
7	$5.2 \times 10^7$	$5.2 \times 10^7$	4	5	5
8	$3.4 \times 10^8$	$3.4 \times 10^8$	3	4	4
9	$5.1 \times 10^9$	$5.1 \times 10^9$	3	2	2
10	$1.6 \times 10^{10}$	$1.5 \times 10^{10}$	3	1	1
11	$1.0 \times 10^{11}$	$-3.6 \times 10^{10}$	2	0	0 S
12	$1.2 \times 10^{12}$	$-1.8 \times 10^{11}$	2	0	0 S

S: numerically singular matrix.

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VIII-3. Application to Algebraically Singular Matrices

We have processed more than ten thousand matrices on the CDC 7600 computer with order of magnitude varying from 2 to 100, the coefficients  $a_{ij}$ , drawn at random being the orders of magnitude between  $10^{-6}$  and  $10^{+6}$ . One has found these singular matrices by replacing the last line with the sum of the other lines.

The permutation-perturbation method has always made it possible to draw a conclusion as to the singularity of these matrices. Table III shows that this result has been obtained using a number of  $A_1$  elements, never exceeding 3. On the other hand, the higher the order, the more the mean number of necessary elements tends toward 2.

IX. Conclusion

The permutation and perturbation method has always given satisfaction and has never been defective and therefore one can designate it as certain. On the other hand, from this study it stands out that:

Table III

Order of matrices	Number of elements $\Delta$			
	1	2	3	$\geq 4$
2	0%	77%	23%	0%
3	7%	88%	5%	0%
4	6%	89%	5%	0%
5	5%	91%	4%	0%
10	2%	95%	3%	0%
20	1%	96%	3%	0%
50	1%	96%	3%	0%
100	0%	97%	3%	0%

--when the matrix is not numerically singular, a population of 3 or 4 elements is sufficient to assure and know the numerical conditioning of the matrix.

--when the matrix is numerically singular, its singularity is generally found from a population of two elements.

One can then say that this method is certain and efficient. It can be used for numerous problems of linear algebra. Also, it makes it possible to control the intrinsic value  $\lambda$  of matrix  $M$  verifying that the  $M-\lambda I$  matrix is singular.

Applied here to a problem of linear algebra, this method can be generalized for cases of nonlinear algebra because its concept basically is to execute the same algorithm many times propagating the errors in various ways finally to obtain results which vitiate the various errors.

This generalization consists of:

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--on the one hand, changing the order of conducting elementary operations (permutation),

/81

--on the other hand, taking its value by deficiency or excess (perturbation) as the result of each elementary operation.

It permits introducing a new concept of computers making them capable of combining an estimate of their precision in the total results.

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