JOURNAL OF

THE

INDIAN INSTITUTE OF SCIENCE

VOLUME 49 APRIL 1967 NUMBER 2

ON NUMERICAL MEASURES OF SINGULARITY OF A MATRIX

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(Received on October 20, 1966)

ABSTRACT

Three measures for the singularity of near singular matrices have been suggested. One based on the basic principle of linear dependence of the column (or row) vectors constituting the matrix, while the other two on methods of Orthonormalization[17] and Orthogonalization[17], respectively. The advantage of the first measure is the computational ease (as well as greater accuracy in the case of unsymmetric matrics), for instance, in comparison to Neumann-Goldstine's measure. The important feature of the remaining two measurers is that they are part of the inversion proces itself in contrast to those suggested by Turing, Neumanm and Goldstine, all of which involve calculations additional to the task of inversion. Moreover these measures, unlike the suggested measures of Turing, Neumann and Goldstine, do not assume any knowledge of inverse or characteristic values of the matrix and also take into cosideration the degree of accurancy of the elements of the matrix. However in the case of a large matrix, say, of 100 or more order, the second measure based on Orthonormalization method may be impractical and sometimes even not feasible, but the third one based on Orthogonalization method is immune to such difficulty and is, moreover, superior to other measures as actually proved by Numerical examples.

INTRODUCTION

A matrix is said to be singular if its determinant vanishes. And if a matrix possesses a very small determinant value, it is said to be near singular[8] and 'ill conditioned[1] with respeet to inverse'. There is a very large class of problems which give rise to a very highly ill-conditioned matrices. However, speaking about near singular matrices, the well known *Hilbert's* matrices naturally come to mind as typical examples. These matrices are strictly non singular in the theoretical sense, though may appear as singular when their reciprocals are computed numerically. A question arises naturally: 'What is the criterion of deciding whether a matrix is to be taken as singular in the numerical sense?' The answer is a relative one, related to the degree of precision adopted in numerical camputation, particularly with the numerical definition of 'zero'. The usual practice of numerical analysis is to express a number correct up to a finite number of decimal places and to retain these number of decimal places in all subsequent computations. For example, the number $1/6 = 0.16667$ when expressed correct up to five decimal places. Any number which is less than 0.000005 in magnitude has to be neglected and treated as 'zero'. Consequently, the numerical 'zero' in this case is any number less than $1/2 \times 10^{-5}$. If we take the determinant of a matrix to be the measure of singularity and if that determinant turns out to be less than $1/2 \times 10^{-5}$, an obvious conclusion will be that the matrix is to be treated as singular. On the other hand, if the latent root is taken to be the measure of singularity and then if the smallest latent root is less than $1/2 \times 10^{-5}$, the matrix is to be taken as singular. The thing does not end here. If the computations are carried out correct up to, say, eight decimal places, then any number less than $1/2 \times 10^{-8}$ is taken as a numerical zero and if the determinant or the smallest latent root is greater than $1/2 \times 10^{-8}$, the matrix is not singular. Consequently, the numerical definition of singularity is a relative one directly linked with the degree of precision of the computations. Even a truly singular matrix, for example, one whose row sum or column sum is exactly 0, may not turn out to be singular computationally, if the computations are done with more decimal places than the elements of the matrix are expressed. A measure of such singularity of matrices is, therefore, necessary not only to decide whether a matrix should, in the numerical sense, be considered singular or not, but also to have a comparative study of matrices, ill-conditioned with respect to inverse.

The present study is aimed at finding an index to measure the extent of this near singularity for a given matrix taking into account the measure of accuracy in expressing the elements of the matrix. Three methods, for obtaining such an index, are suggested and the merits and demerits of these methods along with those of the existing ones have been discussed thereafter by considering a few numerical examples. Among these three suggested measures, the first one is based on the basic principle of linear dependence of column (or row) vectors of a matrix, the second on Orthonormalization[17] method and the third on Orthogonalization[17] method (without normalization of the orthogonal vectors). The superiority of the last method over the other two and also the existing ones has been demonstrated with numerical examples. It is an added advantage that the latter two methods[17] give the inverse of a matrix. The effect of row and column permutation over these suggested measures has also been shown by considering a few numerical examples.

METHODS

Method 1—(Method based on linear dependence)

The ultimate cause of singularity of a matrix is the linear dependence of its column (or row) vectors. Mathematically n column vectors $a_1, a_2, \cdots, a_n$ of a matrix A of order n are said to be linearly dependent over a field F, provided there exist n elements $x_1, x_2, \cdots, x_n$ of F, not all zero, such that

$$\mathbf{a}_1 x_1 + \mathbf{a}_2 x_2 + \cdots + \mathbf{a}_n x_n = 0 \tag{i}$$

otherwise the n column vectors are said to be linearly independent.

Numerically speaking this is directly linked with the numerical definition of 'zero'.

If the elements of the said matrix are expressed correct up to p decimal places, then numerically the linear dependence of these column vectors means that these column vectors of the matrix numerically satisfy a linear equation, that is to say, the linear expression on the left side of (i) is less than $1/2 \times 10^{-p}$ in magnitude. Or, in other words if

$$\text{mod}\,(x_1 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \cdots + x_n \mathbf{a}_n) < \tfrac{1}{2} \times 10^{-p}$$

the matrix A is singular in the numerical sense. Let us denote by $\vec{\epsilon}$ the vector

$$x_1 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \cdots + x_n \mathbf{a}_n,$$

then

$$\| \vec{\epsilon} \| < \tfrac{1}{2} \times 10^{-p}$$

Theoretically the equation $x_1 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \cdots + x_n \mathbf{a}_n = \vec{\epsilon}$ or $A\mathbf{x} = \vec{\epsilon}$ where $\mathbf{x}\,(= [x_1, x_2, \cdots, x_n]')$ is a column vector, can always be solved for x's provided the matrix A is non-singular and $\vec{\epsilon}$ is given. This does not help much as knowledge of $\vec{\epsilon}$ is not available. The minimum of $\vec{\epsilon}$ can be determined from least square method, as

$$|\vec{\epsilon}|^2 = \mathbf{x}' A' A \mathbf{x} = \text{minimum}$$

where A' = transpose of the matrix A and $\mathbf{x}'$ = transpose of the column vector $\mathbf{x}$. But by choosing x's arbitrarily small, one can make $|\vec{\epsilon}|^2$ as small as one desires irrespective of the elements of A. Hence the need of finding min $|\vec{\epsilon}|^2 / |\mathbf{x}|^2$ is obvious $(\mathbf{x} \neq 0)$.

$$\min \frac{|\vec{\epsilon}|^2}{|\mathbf{x}|^2} = \min \frac{\mathbf{x}' A' A \mathbf{x}}{|\mathbf{x}|^2}$$

$$= \text{smallest latent root of } A' A$$

$$= \mu \text{ (say)}$$

If the matrix A is singular $\mu = 0$. Thus the smallest latent root of $A' A$ is a measure of the singularity of the matrix A or more precisely its square root. If $\sqrt{\mu} < \frac{1}{2} \times 10^{-p}$, then the matrix becomes singular in the numerical sense. It is easy to determine numerically the smallest latent root of $A' A$ by an iteration method such as Jacobi's since $A' A$ is symmetric and positive definite. But this is another computation problem different from inversion.

Method 2—(Grams' Orthonormalization process)

Let $A = (a_1, a_2, \cdots, a_n)$ where $a_i = (a_{1i}, a_{2i}, \cdots, a_{ni})$ denote the column vectors of the matrix A.

From the column vectors $a_1, a_2, \cdots, a_n$, we form orthonormal vectors $z_1, z_2, \cdots, z_n$ which are mutually orthogonal and the norm of each vector is unity.

z_1 can be given by $z_1 = \dfrac{a_1}{|a_1|}$,

$$z_2 \text{ by } z_2 = \frac{a_2 - (a_2\, z_1)\, z_1}{\{|a_2|^2 - (a_2\, z_1)^2\}^{1/2}}$$

In general, the orthonormal vector z_s can be given by

$$z_s = \frac{a_s - \sum\limits_{i=1}^{s-1} (a_s\, z_i)\, z_i}{\{|a_s|^2 - \sum\limits_{i=1}^{s-1} (a_s\, z_i)^2\}^{1/2}}$$

where $(a_s\, z_i)$ denotes the inner product of the s-th column vector of A and i-th column vector of Z where

$$Z = (z_1, z_2, \cdots, z_n)$$

Bessel's Inequality[4]

$$D_s = |a_s|^2 - \sum_{i=1}^{s-1} (a_s\, z_i)^2 \geq 0$$

provides a criterion for deciding whether a particular column vector a_s is linearly dependent on the column vectors $a_1, a_2, \cdots, a_{s-1}$. If a_s is linearly dependent on $z_1, z_2, \cdots, z_{s-1}$, that is to say on $a_1, a_2, \cdots, a_{s-1}$, the Inequality becomes an Equality, *viz.*,

$$|a_s|^2 - \sum_{i=1}^{s-1} (a_s\, z_i)^2 = 0$$

If the original elements of the matrix are expressed correctly up to n decimal places, the numerical zero will be any number $< \frac{1}{2} \times 10^{-n}$.

In Bessel's Inequality, if

$$\left\{|a_s|^2 - \sum_{i=1}^{s-1} (a_s z_i)^2\right\}^{1/2} = x \cdot 10^{-r} \text{ (say)},$$

where $1 \leq x < 10$, the Index of linear dependence I is defined as

$$I_s = \tfrac{1}{2} \cdot 10^{-n} \div x \cdot 10^{-r} = \frac{1}{2x} \cdot 10^{r-n}$$

For actual linear dependence $I \geq 1$. If $I < 1$, there is no linear dependence in the strict sense, but I will give a measure of linear dependence and thus of near singularity.

Method 3—(Orthogonalization Method)

This method involves the formation of the Orthogonal basis of the matrix A without normalization of the Orthogonal vectors $x_1, x_2, \cdots, x_n$. Generally we can write

$$x_{s+1} = a_{s+1} - \sum_{i=1}^{s} \frac{a_{s+1}\, x_i}{|x_i|^2} x_i$$

In case a_{s+1} is linearly dependent on the preceding vectors $a_1, a_2, \cdots, a_s$, $|x_{s+1}|^2$ will vanish, *i.e.*, the norm of $x_{s+1} = 0$. In this case we define the Index in the following way.

If norm of $x_{s+1} = x \cdot 10^{-r}$ where $1 \leq x < 10$ and we express the original elements of the matrix in n decimal places, the Index J will be

$$J = \tfrac{1}{2} \cdot 10^{-n} \div x \cdot 10^{-r} = \frac{1}{2x} \cdot 10^{r-n}$$

The two methods are essentially the same, only the second method avoids the rounding off errors of extracting square-roots.

COMPARISON WITH OTHER MEASURES

Turing[1] suggested two measures, *viz.*,

$$M(A) = n \max_{i,j} |a_{ij}| \max_{i,j} |a_{ij}|^{-1}$$

$$N(A) = n^{-1} \text{ norm } A \text{ norm } A^{-1}$$

But both of these assume the knowledge of reciprocal matrix, which cannot be obtained numerically in the majority of the cases. Because inversion process cannot proceed when the condition of the matrix is bad. This is of pure theoretical interest.

John Von Neumann and Goldstine[2] suggested the following measure

$$P(A) = \frac{|\lambda(A)|}{|\mu(A)|}$$

where $\lambda(A)$ is the largest and $\mu(A)$ is the smallest of the latent roots of A.

The largest and smallest latent roots of A are to be calculated which is feasible in many cases, though for unsymmetric matrices, the calculations of λ and μ become tedious and a problem by itself. The first measure, that is, the square-root of the smallest latent root of $A'A$ is easier than Neumann and Goldstine's measure to compute (because $A'A$ is always symmetric even if A is unsymmetric) and can always be computed with accuracy.

The Index I or J, however, is still easier than the first measure to compute because when the reciprocal of the ill-conditioned matrix is computed by the Orthogonalization method[17] or Orthonormalization method, these Indexes are automatically calculated, practically no separate calculations are necessary.

I or J differs from these condition numbers essentially in that it takes into consideration the degree of accuracy of the elements of the matrix. Also it does not assume a knowledge of inverse or characteristic values of the matrix. In fact, the inverse cannot be computed in most cases.

EFFECT OF ROW AND COLUMN PERMUTATION ON THE SUGGESTED MEASURES

In the case of symmetric matrices changing of rows into corresponding columns or *vice versa* has no effect on any of the proposed measures. Under row and column permutation, a symmetric matrix generally turns out to be unsymmetric in most of the cases. Speaking of the unsymmetric matrices as well as symmetric ones, the first measure *i.e*, the one based on the square-root of the smallest latent root of $A'A$ will remain invariant under row and column permutation.

In the Orthogonalization process for inversion, the quantity

$$P = \prod_{i=1}^{n} |x_i|$$

remains invariant under row and column permutation, so that one may look upon P as a measure of the singularity of the matrix; but in majority of the cases (like the suggested measures of Turing[1]) P may not be obtainable because the process of finding $|x_i|$, $i = 1, 2, \cdots, n$ is unable to proceed if a particular column (or row) vector a_{m+1} $(m < n)$ is numerically linearly dependent on the preceding vectors, since in such a case $|x_{m+1}|$ becomes zero numerically and consequently the remaining vectors $x_{m+2}, x_{m+3}, \cdots, x_n$ which have respectively $|x_{m+1}|$, $|x_{m+2}|$, $|x_{m+3}|, \cdots$ as their denominators, cannot be derived.

This difficulty is sure to lead one to consider the quantity $|x_{m+1}|$ which is the only cause for stopping the process, as a measure of singularity. Though not always invariant under row and column permutation, such a measure based on $|x_{m+1}|$, however, tends to be invariant as the matrix approaches singularity and remains invariant when the matrix is numerically singular. This has been shown by considering a few numerical examples.

Measure based on Orthonormalization process is essentially the same as that based on Orthogonalization process, except that the latter measure avoids rounding off errors of extracting square-roots and so the effect of row and column permutation has the same nature as that on the measure based on Orthogonalization method.

Numerical Examples and Programming Aspects

The problem of construction of near singular matrices for testing these methods is made easy by the choice of *Hilbert's* matrices, the linear dependence of the column (or row) vectors becoming more pronounced as we take higher orders.

Scaling: Floating point working is used in all the cases since the range of the numbers handled in these methods is too large for a satisfactory fixed point system. Since the rounding off errors play a significant roll in these cases, retention of a fairly large number of significant digits during the computations becomes necessary.

Checks: The mutual Orthogonality of the column vectors of Z (or $X \equiv [x_1, x_2, \cdots, x_n]$ in the case of the third method) matrix is a sufficient check to determine the accuracy of the calculations. In addition, the normality of the Z-matrix can be checked in the case of the second method.

Results: Numerical examples of 6, 7 and 8 order *Hilbert's* matrices, a singular matrix M of order 7 and two other matrices, each of order 3, are attached and calculations in all the cases were done in floating point with 20 decimal digits unless otherwise stated, to minimize the rounding off errors, and each element of all the *Hilbert's* matrices was retained correct up to 8 significant digits.

Ex. 1 : (HILBERT'S MARTIX OF ORDER 6, METHOD 3 WAS USED)

Using Orthogonal basis of linear transformations of the column vectors of this matrix, mutually orthogonal vectors $x_1, x_2, \cdots, x_6$ were formed, where the smallest of the norms of the orthogonal vectors was given by $|x_6| = 3{\cdot}987 \times 10^{-7}$. According to our previous definition of x and r, the value of $x = 3{\cdot}987$ and $r = 7$. And the Index of linear dependence or Condition number J was given by $J = {\cdot}1254 \times 10^{-1}$ ($\because n = 8$). To compare method 2 and method 3, the following table can be given.

TABLE

A comparative study of D's and x's of method 2 and method 3.

Method 2 Orthonormalization Basis		Method 3 Orthogonalization Basis
Case 1 (Calculations done with 10 significant digits)	Case 2 (Calculations done with 20 significant digits)	(Calculations done with 20 significant digits)
For z_1, $D_1 = 0{\cdot}14913889 \times 10^1$	$D_1 = 0{\cdot}14913889 \times 10^1$	$\lvert x_1\rvert^2 = 0{\cdot}14913889 \times 10^1$
For z_2, $D_2 = 0{\cdot}19173108 \times 10^{-1}$	$D_2 = 0{\cdot}19173107 \times 10^{-1}$	$\lvert x_2\rvert^2 = 0{\cdot}19173107 \times 10^{-1}$
For z_3, $D_3 = 0{\cdot}91424500 \times 10^{-4}$	$D_3 = 0{\cdot}91424452 \times 10^{-4}$	$\lvert x_3\rvert^2 = 0{\cdot}91424452 \times 10^{-4}$
For z_4, $D_4 = 0{\cdot}23050000 \times 10^{-6}$	$D_4 = 0{\cdot}23067036 \times 10^{-6}$	$\lvert x_4\rvert^2 = 0{\cdot}23067036 \times 10^{-6}$
For z_5, $D_5 = -0{\cdot}9 \times 10$	$D_5 = 0{\cdot}30064028 \times 10^{-9}$	$\lvert x_5\rvert^2 = 0{\cdot}30064028 \times 10^{-9}$
which is a negative number.	$D_6 = 0{\cdot}15890052 \times 10^{-12}$	$\lvert x_6\rvert^2 = 0{\cdot}15890113 \times 10^{-12}$
This is due to rounding off errors rendering further computations impossible as z_5 has as its denominator D_5.		

The smallest of $D's$ as determined in case 2 was given by

$$D_6 = 0.15890052 \times 10^{-12}$$

which agreed nearly with the value of $|x_6|^2$ ($= 0.15890113 \times 10^{-12}$)

showing thereby the more accurate results in determining the Index lies in Orthogonalization basis; this was due to the fact that Orthogonal basis avcids extraction of square roots. Again if the calculations are done in floating point with 10 significant digits, we are not able to find z_5 and z_6 because Bessel's Inequility D_5 or D_6 becomes negative due to rounding off errors making further computations impossible, as z_5 and z_6 have as their demonstrators $\sqrt{D_5}$ and $\sqrt{D_6}$. Such trouble will not come in the case of Orthogonalization method.

VON NEUMANN AND GOLDSTINE'S MEASURE: The largest and smallest latent roots of *Hilbert's* matrix of order 6 are 1.61889971 and 0.00000010 respectively and the measure is

$$P(A) = \frac{1.61889971}{0.00000010} = 1.61889971 \times 10^7$$

and the Index of linear dependence is $1/2 \times 10^{-8} \times P(A) = .80944985 \times 10^{-1}$

Measure on the basis of the smallest latent root of

$$A'A: \sqrt{\mu} = .00000010 = 1 \times 10^{-7}$$

and the Condition number is

$$1/2 \times 10^{-}8. \frac{1}{\sqrt{\mu}} = .5 \times 10^{-1}.$$

Ex. 2: (HILBERT'S MATRIX OF ORDER 7, METHOD 3 WAS USED)

Using Orthogonal basis of linear transformations of the column vectors of the matrix, the mutually orthogonal vectors $x_1, x_2, \cdots, x_7$ were found, where the smallest of the squared norms of the orthogonal vectors was given by $|x_7|^2 = 0.3229408 \times 10^{-15}$ and the norm was given by $|x_7| = 1.797 \times 10^{-8}$ and consequently the Index of linear dependence or Condition Number $J = .3349 \times 10^{\circ}$ and the smallest latent root is 0.00000000.

Ex. 3: (HILBERTS' MATRIX OF ORDER 8, METHOD 3 WAS USED)

In this case also, exactly similarly as above, the mutually orthogonal vectors were formed, where the smallest of the norms of the orthogonal vectors was given by $|x_8| = 8.036 \times 10^{-10}$ and consequently the Condition Number $J = 0.622 \times 10^1 > 1$. Hence this matrix was singular in the numerical sense.

Ex. 4: (A SINGULAR MATRIX OF ORDER 7, METHOD 3 WAS USED)

The singular matrix expressed in 4 decimal places was given by

$$\begin{bmatrix} 1.0000 & -0.4589 & -0.5612 & -0.0201 & -0.3947 & -0.3123 & -0.6412 \\ -0.4589 & 1.0000 & 0.3114 & 0.8525 & 0.0429 & 0.2861 & -0.3190 \\ -0.5612 & 0.3114 & 0.0000 & 0.7502 & -0.0655 & 0.1467 & -0.4462 \\ -0.0210 & 0.8525 & 0.7502 & 1.5826 & -0.4173 & 0.1205 & -0.1240 \\ -0.3947 & 0.0429 & -0.0655 & -0.4173 & 1.0000 & 0.1882 & -0.3511 \\ -0.3123 & 0.2861 & 0.1467 & 0.1205 & 0.1882 & 1.0000 & -0.3092 \\ 0.6412 & -0.3190 & -0.4462 & -0.1240 & -0.3511 & -0.3092 & 1.0000 \end{bmatrix}$$

where the 4th column was the sum of the preceding 3 columns.

Here the smallest of the squared norms of the mutually orthogonal vectors $x_1, x_2, \cdots, x_7$ was given by $|x_4|^2 = 0.48280000 \times 10^{-38}$ and the norm was given by $|x_4| = 6.948 \times 10^{-20}$ and therefore the Condition number $J = .7195 \times 10^{11} >> 1$. Hence this matrix is strictly singular even if the elements of it were expressed correct upto 18 decimal places instead of 4 decimal places.

Ex. 5: (AN UNSYMMETRIC MATRIX OF ORDER 3)

The matrix was given by

$$A = \begin{bmatrix} .2 & .2 & .1 \\ .1 & .3 & .1 \\ .1 & .2 & .2 \end{bmatrix}$$

Here the smallest of the squared norms of the mutually orthogonal vectors x_1, x_2 and x_3 was given by $|x_3|^2 = \cdot 01190476$ and P was given by $P = \sqrt{(\cdot 06 \times \cdot 035 \times \cdot 01190476)} = \cdot 00500000\cdot$

When the first two columns were interchanged, the squared norm of the smallest orthogonal vector x_3 as well as $P[= \sqrt{(\cdot 17 \times \cdot 01235294 \times \cdot 01190476)} = 0\cdot 00500000]$ would remain invariant; but when the last two columns were interchanged, the squared norm of the smallest orthogonal vector x_2 was given by $|x_2|^2 = \cdot 01833333$; and $P(= \sqrt{(\cdot 06 \times \cdot 01833333 \times \cdot 02272727)} = \cdot 00500000)$, of course, would remain invariant as it was.

The smallest latent root of $A' A$ was given by $\cdot 92330317$ and this would be unaffected under row and column permutation of the matrix A.

Ex. 6: (A NEAR SINGULAR MATRIX OF ORDER 3, METHOD 3 WAS USED)

Calculations were done correct upto 7 decimal places. The matrix was given by

$$\begin{bmatrix} \cdot 21 & \cdot 32 & \cdot 45 \\ \cdot 21 & \cdot 32 & \cdot 44 \\ \cdot 67 & \cdot 78 & \cdot 59 \end{bmatrix}$$

The smallest of the squared norms of the mutually orthogonal vectors x_1, x_2 and x_3 was given by $|x_3|^2 = \cdot 500 \times 10^{-4}$ when the columns were changed to corresponding rows, the smallest of the squared norms of the orthogonal vectors would be $|x_2|^2 = \cdot 419 \times 10^{-4}$.

Acknowledgment

The author wishes to express his sincere thanks to Prof. S. K. Mitra of Indian Statistical Institute, Calcutta for his able guidance and to Prof P. L. Bhatnagar of Indian Institute of Science, Bangalore for taking keen interest in the preparation of this paper and for fruitful discussions.

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