ON A DIFFICULTY OF CONSTRUCTING PADÉ APPROXIMATION OF ORDER (n, n) TO THE HYPERGEOMETRIC FUNCTION $F(\alpha, \beta, \gamma; x)$

by S. K. MAJUMDAR *and* M. MANDAL, *Computer Centre, Jadavpur University, Calcutta 32*

(Communicated by F. C. Auluck, F.N.A.)

(*Received 18 March 1975*)

The present investigation shows that the Padé Table of order (n, n) to the hypergeometric function $F(\alpha, \beta, \gamma; x)$ may be difficult to construct for certain sets of values of α, β and γ due to high ill-conditionedness (with respect to inversion) of the relevant matrices. The results of the numerical experiments for two typical sets of values of α, β and γ are reported here.

While investigating the possibility of developing the Padé approximation of order (n, n) to the hypergeometric function $F(\alpha, \beta, \gamma; x)$ the authors needed the inverse of the following symmetric matrix

$$A = \begin{bmatrix} 1 & \frac{\alpha\beta}{1!\,\gamma} & \frac{\alpha(\alpha+1)\beta(\beta+1)}{2!\,\gamma(\gamma+1)} & \cdots & \frac{\alpha(\alpha+1)\ldots(\alpha+n-1)\beta(\beta+1)\ldots(\beta+n-1)}{n!\,\gamma(\gamma+1)\ldots(\gamma+n-1)} \\ \frac{\alpha\beta}{1!\,\gamma} & \frac{\alpha(\alpha+1)\beta(\beta+1)}{2!\,\gamma(\gamma+1)} & & \cdots & \frac{\alpha(\alpha+1)\ldots(\alpha+n)\beta(\beta+1)\ldots(\beta+n)}{(n+1)!\,\gamma(\gamma+1)\ldots(\gamma+n)} \\ \vdots & & & & \vdots \\ \frac{\alpha(\alpha+1)\ldots(\alpha+n-1)\beta(\beta+1)\ldots(\beta+n-1)}{n!\,\gamma(\gamma+1)\ldots(\gamma+n-1)} & & & \cdots & \frac{\alpha(\alpha+1)\ldots(\alpha+2n)\beta(\beta+1)\ldots(\beta+2n)}{(2n+1)!\,\gamma(\gamma+1)\ldots(\gamma+2n)} \end{bmatrix}$$

The inverse building by standard numerical techniques created difficulties even when the order of A was 7. It was found that the elements of the inverse matrix were extremely sensitive to small changes in the elements a_{ij} of the matrix A. This is shown in the following example where $\alpha = \beta = \frac{1}{2}$, $\gamma = 5/2$. All numerical computations are done on an IBM 1130 computer using extended precision arithmetic. With the above values of (α, β, γ) the matrix A with $n = 7$ becomes

$B =$

0·1000000 (+01)	0·10000000 (00)	0·32142857 (−01)	0·14880952 (−01)	0·82859848 (−02)	0·51628059 (−02)	0·34705528 (−02)
0·1000000 (00)	0·32142857 (−01)	0·14880952 (−01)	0·82859848 (−02)	0·51628059 (−02)	0·34705528 (−02)	0·24643841 (−02)
0·32142857 (−01)	0·14880952 (−01)	0·82859848 (−02)	0·51628059 (−02)	0·34705528 (−02)	0·24643841 (−02)	0·18239685 (−02)
0·14880952 (−01)	0·82859848 (−02)	0·51628059 (−02)	0·34705528 (−02)	0·24643841 (−02)	0·18239685 (−02)	0·13945156 (−02)
0·82859848 (−02)	0·51628059 (−02)	0·34705528 (−02)	0·24643841 (−02)	0·18239685 (−02)	0·13945156 (−02)	0·10943916 (−02)
0·51628059 (−02)	0·34705528 (−02)	0·24643841 (−02)	0·18239685 (−02)	0·13945156 (−02)	0·10943916 (−02)	0·87750310 (−03)
0·34705528 (−02)	0·24643841 (−02)	0·18239685 (−02)	0·13945156 (−02)	0·10943916 (−02)	0·87750310 (−03)	0·71635670 (−03)

The number in the parantheses should be read as exponents, i.e., 0·34705528 (−02) is $0{\cdot}34705528 \times 10^{-2}$. Consider now the linear system of equations.

$$B \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \end{pmatrix} \begin{matrix} = 0{\cdot}11639431\ (+01) \\ = 0{\cdot}16640753\ (\ 00) \\ = 0{\cdot}68231505\ (-01) \\ = 0{\cdot}37483163\ (-01) \\ = 0{\cdot}23696603\ (-01) \\ = 0{\cdot}16288121\ (-01) \\ = 0{\cdot}11841672\ (-01) \end{matrix}$$

The exact solution of this system is $x_1 = x_2 = x_3 = x_4 = x_5 = x_6 = x_7 = 1$. When only b_{45} is increased by 0·0005 the solution becomes

$x_1 = 0{\cdot}9999604$ $\qquad x_5 = -0{\cdot}0000124$

$x_2 = 1{\cdot}0050291$ $\qquad x_6 = 2{\cdot}0619296$

$x_3 = 0{\cdot}9211478$ $\qquad x_7 = 0{\cdot}5840395$

$x_4 = 1{\cdot}4245934$

Further, the element a_{ij} of A is given by

$$a_{11} = 1$$

$$a_{ij} = \frac{\alpha(\alpha+1)\ldots(\alpha+i+j-3)\ \beta(\beta+1)\ldots(\beta+i+j-3)}{(i+j-2)!\ \gamma(\gamma+1)\ldots(\gamma+i+j-3)} \quad (i+j \geqslant 3)$$

$$= \frac{\Gamma(\gamma)}{\Gamma(\alpha)\ \Gamma(\beta)} \cdot \frac{\Gamma(\alpha+i+j-2)\ \Gamma(\beta+i+j-2)}{\Gamma(\gamma+i+j-2)}.$$

We were interested in the cases (i) $\alpha = \beta = \frac{1}{2}$, $\gamma = 5/2$ and (ii) $\alpha = 5/2$, $\beta = \frac{1}{2}$, $\gamma = 7/2$.

For case (i),

$$a_{ij} = \frac{\Gamma(5/2)}{\Gamma(\frac{1}{2})\Gamma(\frac{1}{2})} \cdot \frac{\Gamma(i+j-3/2)\ \Gamma(i+j-3/2)}{(i+j-2)!\ \Gamma(i+j+\frac{1}{2})}$$

$$= \frac{\Gamma(5/2)}{\Gamma(\frac{1}{2})\ \Gamma(\frac{1}{2})} \cdot \frac{(i+j-5/2)(i+j-7/2)\ldots 3/2 \cdot \frac{1}{2}\Gamma(\frac{1}{2})(i+j-5/2)\ldots\frac{1}{2}\Gamma(\frac{1}{2})}{(i+j-2)!\ (i+j-\frac{1}{2})\ (i+j-3/2)\ldots\frac{1}{2}\Gamma(\frac{1}{2})}$$

$$< \frac{\Gamma(5/2)}{\Gamma(\frac{1}{2})} \cdot \frac{(i+j-2)\ (i+j-3)\ldots 1}{(i+j-2)!\ (i+j-\frac{1}{2})\ (i+j-3/2)}$$

$$= \frac{\Gamma(5/2)}{\Gamma(\frac{1}{2})} \cdot \frac{1}{(i+j-\frac{1}{2})(i+j-3/2)}$$

In the second case in a similar way

$$a_{ij} < \frac{\Gamma(7/2)}{\Gamma(5/2)} \cdot \frac{1}{i+j-\frac{1}{2}}.$$

Thus in both the cases, when (i,j) are made arbitrarily large, $a_{ij} \to 0$. The elements of the Hilbert matrix behave similarly. In view of the foregoing two observations, namely (i) sensitivity of the elements of A to small changes and (ii) $a_{ij} \to 0$ as (i,j) becomes arbitrarily large, we anticipated that the matrix A may be ill-conditioned with respect to inversion for the particular values of (α, β, γ) chosen. We calculated the eigenvalues of the matrix A for two sets of values of (α, β, γ) when the order of the matrix A is 7, to determine the respective condition numbers. The eigenvalues for both sets of values of (α, β, γ) are given in the following Table.

$\alpha = \beta = \frac{1}{2}$, $\gamma = 5/2$	$\alpha = 5/2$, $\beta = \frac{1}{2}$, $\gamma = 7/2$
0·10117146 (+01)	0·12612565 (+01)
0·32614549 (−01)	0·20854050 (00)
0·30069489 (−02)	0·18853055 (−01)
0·19119393 (−03)	0·95691675 (−03)
0·67699643 (−05)	0·29233083 (−04)
0.13313776 (−06)	0·48579968 (−06)
0·39941330 (−07)	0·32148508 (−07)

The eigenvalues were calculated by Givens' method. To have an estimate of the error in the computed eigenvalues, we have taken Ortega's (1963) error analysis of Householder's reduction to tridiagonal form. According to this, the maximum deviation between the eigenvalues of A and those of the computed tridiagonal matrix is given by

$$\varepsilon_1 \leqslant \frac{f(n)\, 2^{-t} \, \| A \|}{1 - f(n)\, 2^{-t}} \qquad \ldots(1)$$

where

$$\| A \| = \Big(\sum_{i,j=1}^{n} | a_{ij} |^2 \Big)^{1/2}$$

$t =$ number of binary places used in the floating point arithmetic.

$$f(n) = 6n^{3/2} + 286n - 596 \qquad \ldots(2)$$

$n =$ order of the matrix A.

Again the maximum deviation between the eigenvalues of the computed tridiagonal matrix C and those approximated by Sturm sequence process is given by

$$\varepsilon_2 \leqslant \rho \, \| C \| \, 2^{-t} \qquad \ldots(3)$$

where

$$\rho \sim 10$$

Thus a bound for the total error $(\varepsilon_1 + \varepsilon_2)$ can be estimated from (1), (2) and (3). A bound for the total error $(\varepsilon_1 + \varepsilon_2)$ in the computed eigenvalues of A is essentially the bound for the error caused by tridiagonalisation. In our case when $\alpha = \beta = \frac{1}{2}$, $\gamma = 5/2$, the values of ε_1 has been calculated for the matrix of order 7 taking $t = 31$ and we obtained $\varepsilon_1 = 0{\cdot}7151157 \times 10^{-6}$. Hence it is reasonable to conclude that the calculated eigenvalues may be uncertain by a few units in the sixth decimal place. Accepting this uncertainty in the calculated eigenvalues we find that the ratio of the largest to the smallest eigenvalue (condition number) is 10^7. In view of this we conclude that the martix is ill-conditioned with respect to numerical inversion. We observed similar behaviour of the matrix for some other sets of values of (α, β, γ) also. The computations were carried out on an IBM 1130 Computer using extended precision arithmetic.

Reference

Ortega, J. M. (1963). An error analysis of Householder's method for the symmetric eigen value problem. *Numer. Math.*, 5, 211–25.