Introduction to programming in FORTRAN 90

Spring 2016

(1) Write a program to calculate the trace of a 3×3 matrix

    (a) by hardcoding the components of the matrix and the formula for the trace.

    (b) by reading the components of the matrix from an external file and using DO LOOPS

    (c) by writing a subroutine to calculate the trace

(2) Generalize the above program to read in a matrix of arbitrary size and perform a check if it is a square matrix and only then move on to calculating it's

    (a) trace

    (b) determinant

    (c) inverse

    (d) transpose

(3) Write a program to multiply any two matrices of arbitrary size.

(4) Write a program to solve a system of linear equations $Ax=b$. The program should read size of the system n, the coefficient matrix A of size $n \times n$ and RHS vector b of size $n \times 1$ from an input file. The solution vector x should be written to an output file.

Numerical data for verification of the programs

$$A = \begin{bmatrix} 3 & 4 & 8 \\ 1 & 5 & 6 \\ 9 & 4 & 7 \end{bmatrix} \quad A^{-1} = \begin{bmatrix} -0.103 & -0.037 & 0.150 \\ -0.439 & 0.477 & 0.093 \\ 0.383 & -0.224 & -0.103 \end{bmatrix} \quad A^T = \begin{bmatrix} 3 & 1 & 9 \\ 4 & 5 & 4 \\ 8 & 6 & 7 \end{bmatrix}$$

$\det(A) = -107$; $\text{tr}(A) = 15$

$$B = \begin{bmatrix} 6 & 2 & 3 \\ 8 & 9 & 12 \\ 9 & 4 & 7 \end{bmatrix} \quad AB = \begin{bmatrix} 122 & 74 & 113 \\ 100 & 71 & 105 \\ 149 & 82 & 124 \end{bmatrix}$$

Solution to the following system of linear equations is $x_1 = 1, x_2 = -1, x_3 = 2$

$$-x_1 + x_2 + 2x_3 = 2$$
$$3x_1 - x_2 + x_3 = 6$$
$$-x_1 + 3x_2 + 4x_3 = 4$$

This algorithm computes a solution of $f(x) = 0$ given an initial approximation x_0 (starting value of the iteration). Here the function $f(x)$ is continuous and has a continuous derivative $f'(x)$

input : f, f', initial approximation x_0, tolerance $\epsilon > 0$, maximum number of iterations maxiter

output: Approximate solution $x_n, (n \leq maxiter)$ or message of failure

for $n = 0,1,2,3 \dots$ maxiter-1 **do**

    Compute $f'(x_n)$;

    if $f'(x_n) = 0$ **then**

        OUTPUT "Failure". STOP;

        Procedure completed unsuccessfully;

    else

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

    end

    if $|x_{n+1} - x_n| \leq \epsilon$ **then**

        OUTPUT x_{n+1} STOP ;

        Procedure completed unsuccessfully

    end

end

Algorithm 1: Newton's Method for solving equations $f(x) = 0$

(5) Using the above algorithm find the positive solution of $2\sin x = x$. (Solution : 1.89549)

(6) Solve the following simultaneous system of non linear equations using the above Newton-Raphson method

$$x^2 + y^2 = 4$$
$$x^2 - y = -1$$