CS 131 NUMERICAL METHODS
SECOND MACHINE PROBLEM
DUE: SEPTEMBER 4, 2013

PROBLEM DESCRIPTION

'***The purpose of computing is insight, not numbers.***' (R.W. Hamming)

For instance, there is more to solving the linear system $\mathbf{Ax} = \mathbf{b}$ than getting a set of numbers we call the solution vector. Unlike in textbook exercises, in which the coefficients a_{ij} and the constants b_i are 'given' (and usually assumed to be 'exact'), in actual applications these quantities are often the result of measurements or of computations, and are therefore infected with errors (roundoff, truncation, etc.). It is thus pertinent to ask what the effect on the computed solution might be of these errors in the input data. The answer to this question is directly related to the notion of the *conditioning* of the linear system $\mathbf{Ax} = \mathbf{b}$. If the linear system is *well-conditioned*, small errors in $\mathbf{A}$ or $\mathbf{b}$ will have no significant effect on the computed solution; if the linear system is *ill-conditioned*, small errors in $\mathbf{A}$ or $\mathbf{b}$ can make the computed solution completely meaningless.

A measure of the conditioning of the linear system $\mathbf{Ax} = \mathbf{b}$ is the condition number of the matrix $\mathbf{A}$, defined as $cond(\mathbf{A}) = ||\mathbf{A}||\,||\mathbf{A^{-1}}||$, where $||\quad||$ is some matrix norm, such as:

1-norm: $||\mathbf{A}||_1$ = maximum absolute column sum of $\mathbf{A}$

2-norm: $||\mathbf{A}||_2$ = largest *singular value* of $\mathbf{A}$

∞-norm: $||\mathbf{A}||_\infty$ = maximum absolute row sum of $\mathbf{A}$

Frobenius norm: $||\mathbf{A}||_F$ = square root of the sum of the squares of all the elements of $\mathbf{A}$

It is clear that $||\mathbf{A}||_1$, $||\mathbf{A}||_\infty$ and $||\mathbf{A}||_F$ are readily computed. To find $||\mathbf{A}||_2$ we take note of the following facts about $\mathbf{A}$.

1. Any $n \times n$ matrix $\mathbf{A}$ can be written as $\mathbf{USV^t}$ where $\mathbf{U}$ and $\mathbf{V}$ are $n \times n$ orthogonal matrices and $\mathbf{S} = diag(\sigma_1, \sigma_2, \ldots, \sigma_n)$. The quantities $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n \geq 0$ are called the *singular values* of $\mathbf{A}$, and are all non-zero if $\mathbf{A}$ is non-singular. The product $\mathbf{USV^t}$ is called the *singular value decomposition* (SVD) of the matrix $\mathbf{A}$.

2. The singular values of $\mathbf{A}$ are the square roots of the eigenvalues of $\mathbf{A^tA}$.

3. The singular values of $\mathbf{A^{-1}}$ are the reciprocals of the singular values of $\mathbf{A}$.

Putting 1, 2 and 3 together, we see that the condition number of $\mathbf{A}$ measured in the 2-norm is simply

$$cond(\mathbf{A})_2 = ||\mathbf{A}||_2\,||\mathbf{A^{-1}}||_2 = \sigma_1/\sigma_n = \sqrt{\lambda_1/\lambda_n}$$

where λ_1 and λ_n are the largest and smallest eigenvalues of $\mathbf{A^tA}$.

INSTRUCTIONS

Write a FORTRAN program to find the condition numbers of a matrix $\mathbf{A}$ measured in the $1-, 2-, \infty-$ and F$-$ norms. Use the Gauss-Jordan reduction method, in-place version, to find $\mathbf{A^{-1}}$. To find the eigenvalues of $\mathbf{A^tA}$, use the Faddeev-GRSM-Newton combination as implemented in your first MP with one minor modification, viz., you only need to get the largest and smallest roots of the characteristic polynomial of $\mathbf{A^tA}$, and these are positive roots.

For each problem to be solved, program input will consist of a real square matrix $\mathbf{A}$, the tolerance ϵ_G for the Gauss-Jordan reduction method, and the tolerance ϵ_N and *itmax* for Newton's method. *Your program should be able to solve **any number** of problems, with the input read from a **single external file**.* Prompt the user to specify via the keyboard the pathname for the file.

For *each* problem solved, program output should consist of: (a) $\mathbf{A}$, ϵ_G, ϵ_N and $itmax$ (b) the computed $\mathbf{A^{-1}}$ and $det(\mathbf{A})$, and (c) the computed condition numbers of $\mathbf{A}$. **The entire output should be stored in a single external file.**

Test your program using the following test matrices. Use $\epsilon_G = 10^{-10}$, $\epsilon_N = 10^{-10}$ and $itmax = 50$. **Use double precision arithmetic throughout**.

(a) $\begin{bmatrix} 6 & 2 & 1 & -1 \\ 2 & 4 & 1 & 0 \\ 1 & 1 & 4 & -1 \\ -1 & 0 & -1 & 3 \end{bmatrix}$ (b) $\begin{bmatrix} 3 & 8 & 4 & 5 \\ 4 & 9 & 6 & 7 \\ 2 & 5 & 7 & 6 \\ 7 & 7 & 6 & 9 \end{bmatrix}$ (c) $\begin{bmatrix} 12 & 25 & -17 & 33 & 28 & 42 \\ -27 & 35 & 15 & 46 & 57 & 30 \\ 11 & 17 & 34 & 42 & 25 & 55 \\ 44 & 36 & -27 & 52 & 15 & -33 \\ -37 & 45 & 18 & 31 & 23 & 49 \\ 14 & 25 & 34 & 43 & 52 & 41 \end{bmatrix}$

(d) the Vandermonde matrix of size 5

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 4 & 8 & 16 \\ 1 & 3 & 9 & 27 & 81 \\ 1 & 4 & 16 & 64 & 256 \\ 1 & 5 & 25 & 125 & 625 \end{bmatrix}$$

(e) the Hilbert matrix $\mathbf{H}$ of size 4, where $h_{ij} = \dfrac{1}{i+j-1}$

(f) an 8×8 matrix of your choice

You may use the following results to check your MP.

1. For test matrix (c)

   Determinant: 7,243,895,304
   Condition numbers
   1−norm: 37.80
   2−norm: 19.38
   ∞−norm: 33.62
   F−norm: 25.62

2. For test matrix (e)

   Determinant: 0.165344D−06
   Condition numbers
   1−norm: 28,375
   2−norm: 15,430
   ∞−norm: 28,375
   F−norm: 15,614

$$\mathbf{A^{-1}} = \begin{bmatrix} 16 & -120 & 240 & -140 \\ -120 & 1200 & -2700 & 1680 \\ 240 & -2700 & 6480 & -4200 \\ -140 & 1680 & -4200 & 2800 \end{bmatrix}$$

Submit on or before due date: (a) your program (**source and .exe files**) and (b) **test data files** to *epquiwa@gmail.com* using the following format: *lastname_firstname.zip* or *.rar*.

REMINDER (from Course Syllabus) re MP's: *A student with outstanding MP requirements will not be allowed to take the exams. Credit declines at 10 points per calendar day to zero 10 days after due date. The MP's are a requirement for the course; they must be submitted and accepted, whether the student receives credit or not.*

WARNING: To avoid last-minute MP submission before a scheduled exam, no MP will be accepted if submitted within 10 hours of the examination start time. (You should spend this time reviewing for the exam, not rushing your MP.)