Tentamen Numerical Mathematics 2
October 31, 2003

Duration: 3 hours

N.B. Unless stated otherwise, the notation used is as in the book of Burden and Faires.

Problem 1

Consider the Schrödinger equation

$$\frac{\partial u}{\partial t} = i\frac{\partial^2 u}{\partial x^2}$$

for x in $[0,1]$, $t \geq 0$ with $u(0,t) = u(1,t) = 0$ and $u(x,0)$ given. Here i is the imaginary unit.

a. Show that a semi-discretization (discretization in space only) of this Schrödinger equation is given by the system of ordinary differential equations

$$\frac{dv}{dt} = Bv,$$

where

$$\begin{aligned} (Bv)_1 &= i(v_2 - 2v_1)/h^2, \\ (Bv)_j &= i(v_{j+1} - 2v_j + v_{j-1})/h^2 \text{ for } j = 2, ..., m-2, \\ (Bv)_{m-1} &= i(-2v_{m-1} + v_{m-2})/h^2 \end{aligned}$$

with $h = 1/m$, and m a natural number. What is the local truncation error?

b. Locate the eigenvalues of the matrix B defined in part a by Gerschgorin's theorem.

c. Proof the first part of Gerschgorin's theorem that states that the eigenvalues of a matrix are in the union of the Gerschgorin disks.

d. Determine the regions of stability of the Euler method and the Trapezoidal rule and make a sketch of them. Which of these methods is appropriate for the problem in part a?

Problem 2

a. Consider the system

$$\begin{bmatrix} \epsilon & 1 \\ 1 & \epsilon \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

in which ϵ is less than the unit round; so $1+\epsilon$ is rounded to 1 on the computer. Determine the solution of this system with rounding if no pivoting is used. Determine also the exact solution. Use this solution to compute the error in the solution with rounding.

b. Compute the solution of the system in part a with rounding and with partial pivoting and compute again the error. In which step of the elimination process in part a is essential information of the original system lost?

Please turn over!

c. In general, systems are solved by an LU factorization of the matrix using partial pivoting and row scaling. Solve in this way the system

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 5 \\ 6 \end{bmatrix}$$

d. What is a band matrix? What can be said about the structure of the L and U factor of such a matrix if it can be factored without pivoting?

e. In absence of roundoff errors, the conjugate gradient method solves a system $Ax = b$ with A symmetric positive definite (what does this mean?) in at most n steps; here n is the order of the matrix. Explain why this is the case.

Problem 3

a. Let $w, d \in R^m$. Suppose that holds $(I - 2ww^T)d = [\alpha, 0, ..., 0]^T$ with $||w||_2 = 1$ and α a scalar. Give the value of α and show that w is given by

$$w_1 = \sqrt{(1 - d_1/\alpha)/2}, \ w_i = -d_i/(2\alpha w_1) \text{ for } i = 2, ..., m.$$

b. Using an Householder matrix, transform the matrix

$$A = \begin{bmatrix} 1 & 3 & 4 \\ 3 & 1 & 2 \\ 4 & 2 & 0 \end{bmatrix}$$

to tridiagonal form.

c. Describe the QR method for the determination of eigenvalues. Why is there a shift in this method? Why is it beneficial to start off with a tridiagonal matrix?