Numerical Analysis Prelim

January, 2003

TIME: (150 MINUTES) January 14, 2003, 10:30 - 1:00 a.m.

You must complete 4 of the following 6 problems. On the scoring table below, put an X through the problems you do not want to be graded. Only 4 problems will be graded, so do not forget to mark two out. No aids except calculators permitted

NAME:__________________________

For Grader Only	
1	/ 25
2	/ 25
3	/ 25
4	/ 25
5	/ 25
6	/ 25
Σ	/100

1. Multiple roots of pose a number of difficulties for many root finding methods. One way to find multiple roots of $f(x) = 0$ is to define a new function $u(x)$ as:

$$u(x) = \frac{f(x)}{f'(x)} \,.$$

   (a) Develop an alternative form of Newton's method in terms of $f^{(n)}(x)$ for points of multiple roots.

   (b) Show that Newton converges quadratically to a multiple root using $u(x)$.

   (c) Show that $f(x)$ goes to zero faster than $f'(x)$ at a multiple root.

Solution

(a)

$$x_{i+1} = x_i - \frac{u(x_i)}{u'(x_i)}$$

since,

$$u'(x) = \frac{(f'(x))^2 - f(x)\, f''(x)}{(f'(x))^2}$$

then,

$$x_{i+1} = x_i - \frac{f(x_i)\, f'(x_i)}{(f'(x_i))^2 - f(x_i)\, f''(x_i)}$$

(b) We need to show that $u(x)$ has a simple root. This can be accomplished by assuming that $f(x) = (x-c)^p h(x)$, where $h(c) \neq 0$. Then it is easy to see that

$$u(x) = (x-c)\frac{h(x)}{ph(x) + (x-c)h'(x)}$$

so that $u(x)$ has a simple root at c. Standard theorem for newton says the convergence is quadratic.

(c) We need to show that:

$$\lim_{x \to c} \frac{f(x)}{f'(x)} = 0$$

where c is the root. Let the root have multiplicity m, then for $j < m$, $f^{(j)}(c) = 0$ and $f^{m}(c) \neq 0$. Therefore, using L'Hopital's rule $m-1$ times, it can be shown that

$$\lim_{x \to c} \frac{f(x)}{f'(x)} = 0 \,.$$

2. The cumulative normal distribution is defined as:

$$N(y) = \int_{-\infty}^{y} \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-x^2}{2}\right) dx$$

Find $N(1)$ by using an appropriate transformation of variables to write the above integral as an integral over a finite interval and use two intervals of Simpson's (1/3) rule to evaluate it.

Solution We must do a change a variables to change the improper integral to a proper one, but the variable change, $t = 1/x$, is not defined at $x = 0$. Therefore, we must break up the integral into:

$$N(1) = \int_{-\infty}^{-1} \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-x^2}{2}\right) dx + \int_{-1}^{1} \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-x^2}{2}\right) dx$$

(although the choice of -1 is arbitary) now, defining $t = 1/x$ and $dt = \frac{-1}{x^2}dx = -t^2 dx$ gives:

$$N(1) = \int_{-1}^{0} \frac{1}{\sqrt{2\pi t^2}} \exp\left(\frac{-1}{2t^2}\right) dt + \int_{-1}^{1} \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-x^2}{2}\right) dx$$

N.B. the first integrand is not defined at the upper bound.
To save writing, let $f(x) = \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-x^2}{2}\right)$ and $g(t) = \frac{1}{\sqrt{2\pi t^2}} \exp\left(\frac{-1}{2t^2}\right)$. Evaluating the first integral using Simpson's rule gives:

$$I1 = \frac{0.5}{3}(g(-1) + 4g(0.5) + g(0)?)$$

Need to calculate $g(0)$:

$$\begin{aligned}
\lim_{t\to 0} g(t) &= \lim_{s\to\infty} \frac{s}{\sqrt{2\pi}\exp(\frac{s}{2})} \\
&= \lim_{s\to\infty} \frac{2}{\sqrt{2\pi}\exp(\frac{s}{2})} \quad \text{(Using L'Hopital)} \\
&= 0
\end{aligned}$$

Therefore,

$$I1 = \frac{0.5}{3}(g(-1) + 4g(0.5) + 0)$$

and, trivially,

$$I2 = \frac{1}{3}(f(-1) + 4f(0) + f(1))$$

Finally, $N(1) \simeq I1 + I2$.

3. **Gauss Elimination** Let A be a $n \times n$ matrix.

(a) If A is strictly row-wise diagonally dominant, what condition does it satisfy?

(b) Prove that if A is strictly diagonally dominant, it is nonsingular. (Hint: Envoke a familiar Theorem for the placement of the eigenvalues of A.)

(c) Prove that if A is strictly diagonally dominant, then Gauss Elimination can be preformed on A without pivoting.

Solution:

(a) A is said to be strictly row-wise diagonally dominant if

$$|a_{i,i}| > \sum_{j=1}^{n} |a_{i,j}|.$$

(b) If A is strictly row-wise diagonally dominant then no Gershgorin circle contains the origin. Thus, 0 cannot be an eigenvalue of A

(c) See Atkinson, page...for details. Roughly, after elimination of one column of A, we show that the $(n-1) \times (n-1)$ principle submatrix is also strictly diagonally dominant. By induction, Gauss elimination can be carried out on this submatrix without pivoting.

4. **Matrix Theory** Let A be a nonsingular $n \times n$ matrix.

   (a) Find the perturbation matrix E with smallest Frobenius norm such that $A - E$ is singular. (Hint: Recall that the Frobenius norm of E is given by

$$\|E\|_F^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} |e_{i,j}|^2$$

   and consider the singular value decomposition of A.)

   (b) What is the Frobenius norm of E?

Solution: The singular value decomposition of A is

$$A = U \Sigma V^t,$$

where U and V are unitary matrices and

$$\Sigma = \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_n \end{bmatrix},$$

where $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n \geq 0$ are the singular values of A. Since A is nonsingular, we know that $\sigma_n > 0$. Let

$$E = U \begin{bmatrix} 0 & & & \\ & 0 & & \\ & & \ddots & \\ & & & \sigma_n \end{bmatrix} V^t = \mathbf{u}_n \sigma_n \mathbf{v}_n^t,$$

where $\mathbf{u}_n$ and $\mathbf{v}_n$ are the last columns of U and V, respectively. Now $A - E$ looks like A except that the last singular value is now 0.

Since U and V are unitary, their columns have length 1. Thus,

$$\|E\|_F^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} e_{i,j}^2 = \sigma_n^2 \sum_{i=1}^{n} |u_{i,n}|^2 \sum_{j=1}^{n} |v_{j,n}|^2 = \sigma_n^2.$$

Thus $\|E\|_F = \sigma_n$.

5. **ODEs** The stability domain for a p-stage explicit Runge Kutta (ERK) method with $p \leq 4$ is given by

$$r(\xi) = 1 + \frac{\xi}{1!} + \frac{\xi^2}{2!} + \cdots + \frac{\xi^p}{p!}. \tag{1}$$

The Butcher diagram for any 3-stage, third order, ERK method is given by

$$\begin{array}{l|lll} \alpha_1 = 0 & & & \\ \alpha_2 = a & a & & \\ \alpha_3 = b + c & b & c & \\ \hline & \gamma_1 & \gamma_2 & \gamma_3 \end{array}$$

where the unknown variables can be determined from four order conditions. Armed with this information answer the following questions.

(a) For $p = 3$, find the range of the imaginary axis covered by the stability domain.

(b) Using the above diagram write down the algorithm for the explicit RK3 scheme.

(c) Given that one of the order conditions is $\alpha_2^2\gamma_2 + \alpha_3^2\gamma_3 = 1/3$, determine the remaining three order conditions using (1).

Solution:

(a) Find the points where the boundary of stability intersects the imaginary axis, namely

$$\mid r \mid = 1, \qquad \xi = i\eta, \quad \eta \in \mathcal{R}$$

Hence

$$r(\xi) = \left(1 - \frac{\eta^2}{2}\right) + i\eta\left(1 - \frac{\eta^2}{6}\right)$$

and

$$\mid r \mid = 1 \Rightarrow \left(1 - \frac{\eta^2}{2}\right)^2 + \eta^2\left(1 - \frac{\eta^2}{6}\right)^2 = 1$$

This simplifies to

$$\eta^4\left(\frac{\eta^2}{36} - \frac{1}{12}\right) = 0 \Rightarrow \eta = \pm\sqrt{3}$$

Therefore the stability domain covers the imaginary axis between $\pm\sqrt{3}i$.

(b) The interpretation of the Butchers diagram is as follows

$$\begin{aligned} d^{(1)} &= hf(x_n, y_n) \\ d^{(2)} &= hf(x_n + \alpha_2 h, y_n + ad^{(1)}) \\ d^{(3)} &= hf(x_n + \alpha_3 h, y_n + bd^{(1)} + cd^{(2)}) \end{aligned}$$

and

$$y_{n+1} = y_n + \gamma_1 d^{(1)} + \gamma_2 d^{(2)} + \gamma_3 d^{(3)}$$

(c) Find recurrence relation for ERK3 and match with

$$r(\xi) = 1 + \xi + \frac{\xi^2}{2} + \frac{\xi^3}{6}, \quad \xi = h\lambda$$

then

$$\begin{aligned}
y' &:= f(y) \equiv hy \\
d^{(1)} &= \xi y_n \\
d^{(2)} &= \xi(y_n + ad^{(1)}) = \xi(1 + a\xi)y_n \\
d^{(3)} &= \xi(y_n + bd^{(1)} + cd^{(2)}) = \xi(1 + b\xi + c\xi(1 + a\xi))y_n
\end{aligned}$$

Thus

$$y_{n+1} = (1 + \gamma_1\xi + \gamma_2\xi(1 + a\xi) + \gamma_3\xi(1 + b\xi + c\xi(1 + a\xi)))$$

Let $y_n = r^n$ such that

$$r = 1 + (\gamma_1 + \gamma_2 + \gamma_3)\xi + (a\gamma_2 + (b + c)\gamma_3)\xi^2 + ac\gamma_3\xi^3$$

where $\alpha_2 = a$ and $\alpha_3 = b + c$. Thus

$$\begin{aligned}
(\gamma_1 + \gamma_2 + \gamma_3) &= 1 \\
(a\gamma_2 + (b + c)\gamma_3) &= \frac{1}{2} \\
ac\gamma_3 = \frac{1}{6}
\end{aligned}$$

These are the order conditions together with $\alpha_2^2\gamma_2 + \alpha_3^2\gamma_3 = 1/3$. The first conditions is true for all ERK3 schemes, since we must be able to solve $y' = 1, y(0) = 0$.

(d) ¿From the Butchers diagram we see $a = \alpha_2 = 2/3$ and $c = 2/3$. Hence

$$\begin{aligned}
(\gamma_1 + \gamma_2 + \gamma_3) &= 1 && (2) \\
(\frac{2}{3}\gamma_2 + (b + c)\gamma_3) &= \frac{1}{2} && (3) \\
\frac{4}{9}\gamma_3 = \frac{1}{6} & && (4) \\
\frac{4}{9}\gamma_2 + \alpha_3^2\gamma_3 &= \frac{1}{3} && (5)
\end{aligned}$$

This implies $\gamma_3 = 3/8$. ¿From (3) and (5)

$$\begin{aligned}
\tfrac{2}{3}\gamma_2 + \tfrac{3}{8}\alpha_3 = \tfrac{1}{2} \\
\tfrac{4}{9}\gamma_2 + \tfrac{3}{8}\alpha_3^2 = \tfrac{1}{3}
\end{aligned} \quad \Rightarrow \quad \alpha_3(\alpha_3 - \frac{2}{3}) = 0 \quad \Rightarrow \quad \alpha_3 = 0, \frac{2}{3}$$

Therefore

$$\alpha_3 = 0, \gamma_2 = \frac{3}{4} \Rightarrow b = -\frac{2}{3}$$

$$\alpha_3 = \frac{2}{3}, \gamma_2 = \frac{3}{8} \Rightarrow b = 0$$

Using $\gamma_1 = 1 - \gamma_2 - \gamma_3$ gives the final result

$$\begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \gamma_1 \\ \gamma_2 \\ \gamma_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 2/3 \\ 0 \\ -1/8 \\ 3/4 \\ 3/8 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 0 \\ 2/3 \\ 2/3 \\ 1/4 \\ 3/8 \\ 3/8 \end{pmatrix}$$

6. **PDEs**

Consider the following finite difference scheme that solves the heat equation $u_t = \sigma u_{xx}$:

$$u(x, t+k) - u(x, t-k) = \nu[u(x+h, t) - u(x, t+k) - u(x, t-k) + u(x-h, t)]$$

with timestep k, gridspacing h and where $\nu = 2\sigma k/h^2$, $\sigma > 0$.

(a) Determine the accuracy of the scheme and conditions under which it is consistent.

(b) Show that the scheme is unconditionally stable.
Hint: You may use the results that the roots to the quadratic equation $z^2+bz+c = 0$ with b, c real, lie within the unit circle, if and only if, $|c| \le 1$ and $|b| \le 1 + c$.

Solution:

(a) Taylor Expand all terms about $u(x, t)$

$$\begin{aligned} u(x, t+k) &= \sum_{n=0}^{\infty} \frac{k^n}{n!} \frac{\partial^n}{\partial t^n} u(x, t) \\ u(x, t-k) &= \sum_{n=0}^{\infty} (-1)^n \frac{k^n}{n!} \frac{\partial^n}{\partial t^n} u(x, t) \\ u(x+h, t) &= \sum_{n=0}^{\infty} \frac{h^n}{n!} \frac{\partial^n}{\partial x^n} u(x, t) \\ u(x-h, t) &= \sum_{n=0}^{\infty} (-1)^n \frac{h^n}{n!} \frac{\partial^n}{\partial x^n} u(x, t) \end{aligned}$$

Then LHS gives

$$2 \sum_{n=0}^{\infty} \frac{k^{2n+1}}{(2n+1)!} \frac{\partial^{2n+1}}{\partial t^{2n+1}} u(x, t)$$

and RHS gives

$$2\nu \left[\sum_{n=0}^{\infty} \frac{k^{2n}}{(2n)!} \frac{\partial^{2n}}{\partial x^{2n}} - \sum_{n=0}^{\infty} \frac{k^{2n}}{(2n)!} \frac{\partial^{2n}}{\partial t^{2n}} \right] u(x, t)$$

with $\nu = 2\sigma k/h^2$ this gives

$$u_t - \sigma u_{xx} = -\frac{k^2}{3!} u_{ttt} + 2\sigma \frac{h^2}{4!} u_{xxxx} - \sigma \frac{k^2}{h^2} u_{tt} + \cdots$$

hence

$$u_t - \sigma u_{xx} = \mathcal{O}(k^2) + \mathcal{O}(h^2) + \mathcal{O}\left(\frac{k^2}{h^2}\right)$$

So the local trucation error is $e(k, h) = \mathcal{O}(k^2) + \mathcal{O}(h^2) + \mathcal{O}(k^2/h^2)$ and the scheme is consistent iff $e(x, h) \to 0$ as $k, h \to 0$. Thus $k = o(h)$, or $k = ch^p, p > 1$. With this consistency condition the scheme solve the diffusion equation.

(b) The accuracy of the scheme is $\mathcal{O}(k^2/h^2)$.

(c) To determine stability use the Von-Neumann analysis.

$$\begin{aligned} u(x,t) &= \xi^{\frac{t}{k}} e^{i\omega x} \\ u(x,t+k) &= \xi^{\frac{t}{k}+1} e^{i\omega x} \\ u(x,t+k) &= \xi^{\frac{t}{k}+1} e^{i\omega x} \\ u(x+h,t) &= \xi^{\frac{t}{k}} e^{i\omega(x+h)} \\ u(x-h,t) &= \xi^{\frac{t}{k}} e^{i\omega(x-h)} \end{aligned}$$

substitute into scheme

$$(\xi - \xi^{-1}) = \nu \left(e^{i\omega h} + e^{-i\omega h} - \xi - \xi^{-1} \right)$$

or

$$(1+\nu)\xi^2 - (2\nu \cos \omega h)\xi + (\nu - 1) = 0$$

$$\xi^2 - \frac{(2\nu \cos \omega h)}{(1+\nu)}\xi + \frac{(\nu-1)}{(1+\nu)} = 0$$

Using the hint

$$b = -\frac{(2\nu \cos \omega h)}{(1+\nu)}, \qquad c = \frac{(\nu-1)}{(1+\nu)}$$

Therefore it follows

$$|c| \leq 1 \Rightarrow \nu \geq 0.$$

and

$$|b| \leq 1 + c \Rightarrow |\cos \omega h| \leq 1.$$

These statements are always true. The scheme is therefore unconditionally stable.