The Australian National University

Final - First Semester 2013

MATH 3511/MATH 6111 - Scientific Computing

For HPO Students

Important notes:

- Course/lecture notes are allowed. Reading bricks are allowed. Calculators are allowed.
- Answer all 6 questions.
- Questions have different weights. The total point score is 60.
- A good strategy is not to spend too much time on any question. Read them through first and attack them in the order that allows you to make the most progress.
- Write your answers in the script books provided.
- Show **all** of your work. Be neat.
- If you are unable to complete the proof of a theorem in one part of a question, you may assume it is true to answer any remaining parts of the question.
- **You have 15 minutes reading time.**
- **You have 3 hours to complete the exam.**

Question: 1 (*Root Finding Algorithms*) **10P.**

a). Using a calculator, apply the **secant method** to

$$f(x) = x^4 - x - 10,$$

with starting values $x_0 = 1$ and $x_1 = 2$ to obtain the fifth iterate x_5. Based on x_5, write the root of $f(x) = 0$ correct to two decimal places. *(5P.)*

b). Suppose that r is a zero of an arbitrary function f, such that

$$f(r) = f'(r) = 0 \neq f''(r).$$

Show that if f'' is continuous, then in Newton's method we shall have $e_{n+1} \approx \frac{1}{2}e_n$, which means linear convergence. (Note that $e_n = x_n - r$.) *(5P.)*

Turn over for additional questions ...

Question: 2 (*Polynomial Interpolation*) **10P.**

a). Find the Lagrange and Newton forms of the interpolating polynomial for these data:

x	0	1	2
$f(x)$	-1	2	7

Write both polynomials in the form $a + bx + cx^2$ to verify that they are identical as functions. *(4P.)*

b). If we interpolate the function $f(x) = e^{x-1}$ with a polynomial p of degree 12 using 13 Chebyshev points in the interval $[-1, 1]$, what is a good upper bound for $|f(x)-p(x)|$ on that interval? *(3P.)*

c). Are the following functions splines? Give reasons for your answer.

i).

$$f_1(x) = \begin{cases} -x^2 - 2x^3 & \text{if } -1 \leq x \leq 0, \\ -x^2 + 2x^3 & \text{if } 0 < x \leq 1 \end{cases}$$

ii).

$$f_2(x) = \begin{cases} -x^2 - 2x^3 & \text{if } -1 \leq x \leq 0, \\ x^2 + 2x^3 & \text{if } 0 < x \leq 1 \end{cases}$$

(3P.)

Turn over for additional questions ...

Question: 3 (*Numerical Differentiation and Integration*) **10P.**

a). Derive the formula

$$f'''(x) \approx \frac{1}{h^3}[f(x+3h) - 3f(x+2h) + 3f(x+h) - f(x)]$$

for approximating the third derivative of $f(x)$ and find its order of accuracy. *(5P.)*

b). A numerical integration formula on the interval $[-1, 1]$ uses the quadrature points $x_0 = -\alpha$ and $x_1 = \alpha$, where $0 < \alpha \leq 1$:

$$\int_{-1}^{1} f(x)\ dx \approx w_0 f(-\alpha) + w_1 f(\alpha).$$

The formula is required to be exact whenever f is a polynomial of degree 1; show that $w_0 = w_1 = 1$, independent of the value of α. Show also that there is one particular value of α for which the formula is exact also for all polynomials of degree 2. Find this α, and show that for this value of α, the formula is also exact for all polynomials of degree 3. *(5P.)*

Turn over for additional questions ...

Question: 4 (*Linear systems of equations and rounding errors*) **12P.**

a). Derive an upper bound for the floating point error which occurs when the expression $y = x_1 + (x_2 - x_3)$ is computed using 64 bit IEEE floating point arithmetic. Consider the case where the x_i are any real numbers and apply the model discussed in the lectures. Give the bound in terms of the machine ϵ.

Consider the special case where $x_1 = 0.5$, $x_2 = 0.625$ and $x_3 = 0.6$. Show how you can improve the previously obtained general error bound for this special case.

(5P.)

b). Derive the condition number of the inverse A^{-1} using the condition number κ_A of the matrix A. *(2P.)*

c). Given the linear system of equations

$$\begin{bmatrix} 5 & -1 \\ -1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 7 \\ 4 \end{bmatrix}.$$

Write down the formula of the SOR method for x_1^{k+1} and x_2^{k+1} at the $(k+1)$th step of the iterations. Calculate the optimal relaxation factor in this SOR method. *(5P.)*

Turn over for additional questions ...

Question: 5 (*Ordinary differential equations*) **9P.**

a). Derive the amplification factor for Heun's method. How is the region of A-stability defined for Heun's method? What is the largest set of real numbers contained in this region of A-stability? (Hint: The largest set is an open interval (a, b).) *(4P.)*

b). Consider the one-step method defined by

$$x_{k+1} = x_k + h\, f\left(t_k + \frac{h}{2},\, x_k + \frac{h}{2} f(t_k, x_k)\right).$$

Assume that $f(t, x)$ satisfies a Lipschitz condition in the variable x. What is the convergence order of this method? Prove this convergence rate by showing the conditions given in the lectures. *(5P.)*

Turn over for additional questions ...

Question: 6 (*Discrete Fourier transforms*) **9P.**

a). Let $x = (x_0, \dots, x_{n-1})^T$ and $y = (y_0, \dots, y_{n-1})^T$ be real vectors such that $y_0 = x_0$ and $y_k = x_{n-k}$ for $k = 1, \dots, n-1$. Furthermore let F_n be the discrete n by n Fourier transform matrix introduced in the lectures. Show that the Fourier transform of y is

$$F_n y = \overline{F_n x}$$

where $\overline{F_n x}$ is the component-wise conjugate complex of the Fourier transform $F_n x$.

(3P.)

b). Determine the squares of the Fourier matrices F_2^2 and F_4^2. Prove a formula for F_n^2 for general Fourier matrices F_n. *(4P.)*

c). Use matrix factorisation to write F_8 in terms of F_4. *(2P.)*