The Australian National University

Final - First Semester 2013

MATH 3511 - Scientific Computing

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). Consider an arbitrary smooth function f and define $f_n = f(x_n)$, $f_n' = f'(x_n)$ and $f_n'' = f''(x_n)$. When **Newton's method** is applied to the function $f/\sqrt{f'}$, show that the iteration formula

$$x_{n+1} = x_n - \frac{2 f_n\, f_n'}{2(f_n')^2 - f_n\, f_n''}$$

is obtained. *(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). Determine the values of α, β, and γ, such that the numerical integration formula

$$\int_{-1}^{1} f(x)\, dx \approx \alpha f(-\tfrac{1}{2}) + \beta f(0) + \gamma f(\tfrac{1}{2})$$

is exact for all polynomials of degree ≤ 2. *(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. *(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? Explain in detail (without actually doing the proof) what you would need to verify in order to prove the convergence rate. *(5P.)*

Turn over for additional questions ...

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

a). Let $x = (x_0, \ldots, x_{n-1})^T$ and $y = (y_0, \ldots, y_{n-1})^T$ be real vectors such that $y_0 = x_0$ and $y_k = x_{n-k}$ for $k = 1, \ldots, n-1$. 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. What theorem would you use to derive a formula for the squares F_n^2 for general Fourier matrices F_n? *(4P.)*

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