The Australian National University

Final Exam – June 2014

MATH 3511/MATH 6111 – Scientific Computing

For HPO Students

Important notes:

- Course/lecture notes are allowed. Any notes (handwritten or printed) or copies of notes 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 (*Differentiation*) **8P.**

Determine the coefficients a_0, a_1, a_2 which guarantee that the finite difference formula

$$D(f,h) = a_0 f(0) + a_1 f(h) + a_2 f(2h)$$

gives $D(f,h) = f'(0)$ (the first derivative of f) if f is any second degree polynomial.

Turn over for additional questions ...

Question: 2 (*Polynomial Interpolation*) **12P.**

a) Horner's rule provides a fast way to evaluate the function values $p(x)$ of polynomials p given by

$$p(x) = a_0 + a_1 x + \cdots + a_n x^n.$$

Show how to use the idea of Horner's method to evaluate the Newton form

$$p(x) = c_0 + c_1(x - x_0) + \cdots + c_n(x - x_{n-1}) \cdots (x - x_0)$$

fast. How many multiplications, additions and subtractions would this method require?

(3P.)

b) Assume that $p_n(x)$ is a polynomial which interpolates a smooth function f at the points $x_k = kh$ and $y_k = f(x_k)$ ($h = 1/n$ and $k = 0, \ldots, n$). Recall the interpolation error bound considered in the course and discuss where the values of this bound can be large for this problem. As a large error bound points to large errors it is important to find a way to improve the quality of the interpolation. Describe how to modify the above interpolation problem to get a polynomial with a guaranteed uniform (small) error over the interval.

(4P.)

c) Consider the interpolation problem with 8 interpolation points $x'_k = 0, h, 2h, \ldots, 7h$. Here you should consider the impact a specific reordering of the interpolation points has. In particular, let $x_0 = 0, x_1 = 4h, x_2 = 2h, x_3 = 6h, x_4 = h, x_5 = 3h, x_6 = 5h, x_7 = 7h$. Then let p_7 be the polynomial of degree 7 be such that $p_7(x_k) = y_k$ ($= f(x_k)$) for $k = 0, \ldots, 7$. How does this polynomial p_7 and the error $f - p_7$ compare to the polynomial q_7 and its error $f - q_7$. Here q_7 interpolates f at the original points $x'_k = kh, y'_k = f(x'_k)$.

How do the Lagrangian and Newtonian forms of p_7 and q_7 compare?

Hint: Recall the result about the uniqueness of polynomial interpolation.

(3P.)

d) Show that in the process of computing the Newtonian form of the interpolant for the permuted points one gets a fourth order interpolant which interpolates at the points $0, 2h, 4h, 6h$. *(2P.)*

Turn over for additional questions ...

Question: 3 (*Newton's method*) **12P.**

a) Show that there exists an $x^* \in (0, \pi/2)$ such that $f(x^*) = 0$ where the function f is

$$f(x) = \cos(x) - x.$$

(3P.)

b) What is the iteration step for Newton's method applied to the equation

$$\cos(x) - x = 0?$$

(2P.)

c) Recall that Newton's method is locally second order, i.e., there is a constant $C > 0$ such that

$$|e_{n+1}| \leq C|e_n|^2.$$

Determine the value of C if you assume that $|e_n| \leq 1/2$. *(3P.)*

d) Use the Taylor remainder theorem to show that for all $x \in (0, \pi/2)$ one has

$$|x^* - x| \leq |\cos(x) - x|.$$

(2P.)

e) Assume that you have shown that for $x_0 = \pi/8$ one has $|x^* - x_0| \leq 1/2$. Show that for all $n = 0, 1, 2, \ldots$ the error satisfies $|e_n| \leq 1/2$ if $x_0 = \pi/8$ and x_n is computed with Newton's method. *(2P.)*

Turn over for additional questions ...

Question: 4 (*Linear multistep method*) **12P.**

a) Choose the coefficients a, b, c, d in the multistep method

$$x_{n+1} = a\,x_n + b\,x_{n-1} + h(c\,f_n + d\,f_{n-1})$$

such that the scheme recovers exact solutions $x(t) = 1$, $x(t) = t^2$, $x(t) = t^3$ and $x(t) = t^4$. As usual, let $t_n = nh$ and $f_n = f(t_n, x_n)$ and x_n is an approximation for $x(t_n)$. *(6P.)*

b) Show that the method defined by

$$x_{n+1} = x_n + h(2f_{n+1} - f_n)$$

is unconditionally stable. *(6P.)*

Turn over for additional questions ...

Question: 5 (*Floating point arithmetic and linear solvers*) **8P.**

a) As $a^2 - b^2 = (a-b)(a+b)$ one may compute the value of this expression by either computing the difference of the squares or, alternatively, by computing the product of the difference with the sum of a and b. These two methods may give different results if done using floating point arithmetic. Give a bound on the relative error for both methods assuming that both a and b are floating point numbers which are very close (such that all occurring differences of floating point numbers can be computed exactly) but not equal. Use the floating point error model given in class. Which of the two methods performs better according to your analysis? *(4P.)*

b) Give the reason why all the elements l_{ij} of the L factor obtained from Gaussian elimination with pivoting satisfy $|l_{ij}| \leq 1$. *(2P.)*

c) The conjugate gradient method uses a different descent direction than the steepest descent method. How is the descent direction computed for the conjugate gradient method? Describe in a sentence or two what the advantage of this choice of descent direction is (compared to the one used for steepest descent). *(2P.)*

Turn over for additional questions ...

Question: 6 (*FFT*) **8P.**

a) Recall the factorisation of the Fourier matrix F_n for even $n = 2m$ into three factors: a butterfly matrix, a matrix involving lower order Fourier matrices and a permutation matrix. Write down this factorisation explicitly and give a formula for the matrix elements for all three factors. How many (real or complex) nonzero elements does the butterfly matrix and the permutation matrix have, respectively? *(3P.)*

b) For F_n with $n = 2^k$ the FFT is obtained by successively repeating this factorisation until the remaining factor only involves F_2. How many butterfly matrices and permutations does the resulting factorisation have? *(2P.)*

c) What is the sum of the number of nonzero elements of all the butterfly matrices? If any butterfly matrix occurs multiple times include the total number of nonzeros of all the occurring instances. *(3P.)*

Comment for b) and c): you should include the final factor (in the FFT factorisation) involving only F_2 to the count of butterfly matrix factors. Do this both for the count of factors and for the count of nonzero elements.