NAME OF CANDIDATE: . . . .
STUDENT NUMBER: . . . .

THE UNIVERSITY OF NEW SOUTH WALES

SCHOOL OF MATHEMATICS AND STATISTICS

June 2009

MATH2089
Numerical Methods and Statistics

(1) TIME ALLOWED – 3 Hours

(2) TOTAL NUMBER OF QUESTIONS – 6

(3) ANSWER ALL QUESTIONS

(4) THE QUESTIONS ARE OF EQUAL VALUE

(5) THIS PAPER MAY **NOT** BE RETAINED BY THE CANDIDATE

(6) **ONLY** CALCULATORS WITH AN AFFIXED "UNSW APPROVED" STICKER MAY BE USED

(7) STATISTICAL FORMULAE ARE ATTACHED AT END OF PAPER

Part A – Numerical Methods consists of questions 1 – 3

Part B – Statistics consists of questions 4 – 6

Both parts must be answered

All answers must be written in ink. Except where they are expressly required pencils may only be used for drawing, sketching or graphical work.

Part A – Numerical Methods

1. Answer in a separate book marked Question 1

a) Give the results of the following MATLAB commands. Note that none of the commands is terminated by a semi-colon (;).

i)
```
ans1 = 8 + 3*eps - 8
ans2 = exp(3.2e+120)
ans3 = 0*log(0)
```
ii)
```
A = [1 -3 0; 2 1 -4; 0 0 3]
x = A(:,2)
ans4 = norm(x, Inf)
ans5 = A >= 0
```

b) A simulation of a chemical plant with n processes takes $6n^3 + O(n^2)$ flops. You have a 3GHz dual core PC which can do 2 flops per clock cycle.

i) Estimate the largest simulation that can be run in 10 minutes.

ii) What other factor(s) could limit the size of the simulation?

c) The following MATLAB code generates the given output for a pre-defined real square array A.

```
chk1 = norm(A - A', 1)
chk1 =
     1.4052e-015
ev = eig(A);
evlim = [min(ev) max(ev)]
evlim =
      4.5107e-002   9.1213e+004
```

Giving reasons, answer the following questions.

i) Is A symmetric?

ii) Is A positive definite?

iii) Calculate the 2-norm condition number $\kappa_2(A)$ of A.

iv) When solving the linear system $A\mathbf{x} = \mathbf{b}$, the elements of A and $\mathbf{b}$ are known to 6 significant decimal digits.

A) Estimate the relative error in the computed solution $\bar{\mathbf{x}}$.

B) What confidence do you have in your computed solution?

v) Given the Cholesky factorisation $A = R^T R$, explain how to solve the linear system $A\mathbf{x} = \mathbf{b}$.

2. Answer in a separate book marked Question 2

a) To find the root of a real number, computers typically implement Newton's method. Let $a > 1$ and consider finding the cube root of a, that is $a^{\frac{1}{3}}$.

i) Write this as a polynomial equation $p(x) = 0$.

ii) Show that the interval $[1, a+1]$ brackets a zero of p.

iii) Show that the interval $[1, a+1]$ contains at most one zero of p.

iv) Show that Newton's method can be written as

$$x_{k+1} = \frac{1}{3}\left(2x_k + \frac{a}{x_k^2}\right).$$

v) The method of the previous part was implemented in MATLAB giving the following results

k	e(k)	e(k+1)/e(k)	e(k+1)/e(k)^2	e(k+1)/e(k)^3
1	3.42e+00	4.93e-01	1.44e-01	4.21e-02
2	1.69e+00	3.81e-01	2.26e-01	1.34e-01
3	6.42e-01	2.17e-01	3.38e-01	5.27e-01
4	1.40e-01	6.15e-02	4.41e-01	3.16e+00
5	8.59e-03	4.11e-03	4.78e-01	5.57e+01
6	3.52e-05	1.69e-05	4.81e-01	1.36e+04
7	5.97e-10	7.44e-07	1.25e+03	2.08e+12
8	4.44e-16			

where $e_k = |x^* - x_k|$.

A) What order of convergence do you expect from Newton's method for this problem.

B) Giving reasons, explain if this is achieved or not.

b) Two chemicals are mixed in a stirred tank chemical reactor under controlled conditions to produce a certain product. The problem parameters are

- V = volume of the tank (m^3)
- q = constant flow rate into and out of the tank (m^3/min)
- u_1 = concentration (moles/m^3) of chemical 1
- u_2 = concentration (moles/m^3) of chemical 2
- r = reaction rate (moles/m^3-min)

A mathematical model uses the state variables

- x_1 = concentration of chemical 1 (moles/m^3)
- x_2 = concentration of chemical 2 (moles/m^3)
- x_3 = concentration of product (moles/m^3)

The governing system of ordinary differential equations (ODEs) is

$$\begin{aligned} V\frac{dx_1}{dt} - qu_1 + qx_1 + Vr &= 0 \\ V\frac{dx_2}{dt} - qu_2 + qx_2 + Vr &= 0 \\ V\frac{dx_3}{dt} + qx_3 - Vr &= 0 \end{aligned}$$

and the reaction rate r is assumed to satisfy

$$r = \alpha x_1 x_2$$

where $\alpha > 0$ is constant.

The concentrations of the the two reactants in the constant feed stream is $u(t) = (3.2,\ 4.8)^T$, the flow rate is $q = 10$ m^3/min, the volume of the tank is $V = 2$ m^3 and the reaction rate constant is $\alpha = 2.6$ m^3/mole-min. Initially the mixture in the tank has 5 moles/m^3 of chemical 1 and 3 moles/m^3 of chemical 2, and no product is initially present.

We want to find the concentrations of chemical 1, chemical 2 and the product over a period of 90 seconds.

i) Write this as an initial value problem (IVP) in the standard form

$$\mathbf{x}' = \mathbf{f}(t, \mathbf{x}) \quad t \in [t_0, t_{\max}], \qquad \mathbf{x}(t_0) = \mathbf{y}_0$$

making sure you give **all** the required information.

ii) Write a MATLAB function M-file

```
function f = reaction(t, x)
```

to specify the system of ODEs to be solved. Define any problem parameters required in this function.

iii) Briefly compare and contrast an explicit Euler method and the Runge-Kutta method `ode45` for this problem. Only general features are required, not any explicit calculations.

3. **Answer in a separate book marked Question 3**

The temperature $u(x,t)$ in an insulated wire of length L satisfies the partial differential equation

$$\frac{\partial u(x,t)}{\partial t} = D(x)\frac{\partial^2 u(x,t)}{\partial x^2}, \quad x \in (0,L), \quad t \in (0,T]. \tag{3.1}$$

The conductivity $D(x) > 0$ depends on x as the material changes.

Let u_j^ℓ be the approximation to $u(x_j, t_\ell)$ at the grid points

$$\begin{aligned} x_j &= j\Delta x \quad \text{for } j = 0,\ldots,n+1, \\ t_\ell &= \ell\Delta t \quad \text{for } \ell = 0,\ldots,m, \end{aligned}$$

where $L = (n+1)\Delta x$ and $T = m\Delta t$.

The space grid and the non-zero entries in the coefficient matrix A coming from a discretization of (3.1) are given in Figure 3.1 for $n = 20$.

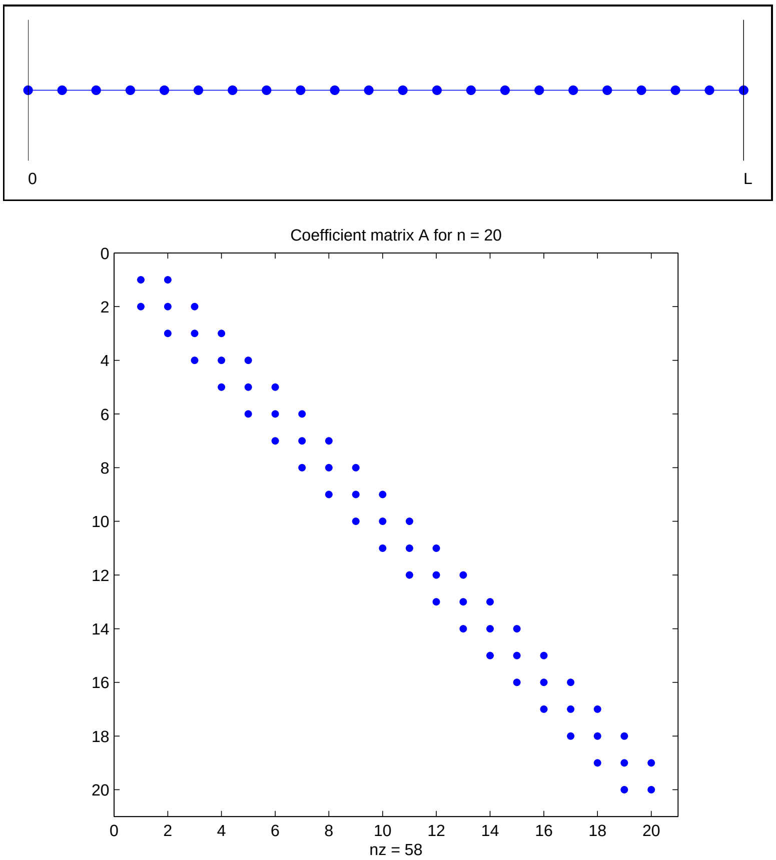

Figure 3.1: Grid and non-zero elements in coefficient matrix

a) What additional information is needed to completely specify this problem?

b) You are **given** the following standard finite difference approximations for a function f of **one** variable:

$$\begin{aligned} f'(x) &= \frac{f(x+h)-f(x)}{h} + O(h), \\ f'(x) &= \frac{f(x+h)-f(x-h)}{2h} + O(h^2), \\ f''(x) &= \frac{f(x+h)-2f(x)+f(x-h)}{h^2} + O(h^2). \end{aligned}$$

At the time step $t_{\ell+1}$ and space point x_j give a

i) central difference approximation of $O(\Delta x^2)$ to

$$\frac{\partial^2 u(x,t)}{\partial x^2},$$

ii) backward difference approximation of $O(\Delta t)$ to

$$\frac{\partial u(x,t)}{\partial t}.$$

c) Using these finite difference approximations, derive the linear equations

$$(2+\alpha_j)u_j^{\ell+1} - u_{j-1}^{\ell+1} - u_{j+1}^{\ell+1} = \beta_j^\ell, \tag{3.2}$$

which determine the unknowns $u_j^{\ell+1}$ for $j = 1, \ldots, n$. Give explicit expressions for α_j and β_j^ℓ.

d) Given that

$$u(0,t) = 40, \quad u(L,t) = 20 \quad t \in (0,T)$$

give the equation (3.2) for a discretization with $n = 20$ at the grid points x_j for

i) $j = 1$;

ii) $j = 14$.

Leave your answer in terms of α_j, β_j^ℓ but make sure you clearly identify what values are known.

e) The linear equations (3.2) can be written in matrix form as $A\mathbf{u}^{\ell+1} = \mathbf{b}^\ell$. You are **not** required to derive the linear system.

i) Calculate the sparsity of A for the case $n = 20$.

ii) Briefly discuss the structure of A that could be exploited to efficiently solve this linear system.