This question paper consists of ?? printed pages, each of which is identified by the Code Number COMP5930M01.

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School of Computing

January 2018

COMP5930M

Scientific Computation

Answer ALL questions

Time allowed: 2 hours

Question 1

A nonlinear system is defined by 2 equations in 2 variables x, y:

$$x^2 y = 2 \tag{1}$$
$$x + y^2 = 1 \tag{2}$$

(a) Formulate the problem as a system of nonlinear equations $\mathbf{F}(\mathbf{U}) = \mathbf{0}$, stating the precise form for $\mathbf{U}$ and $\mathbf{F}(\mathbf{U})$.

Derive the analytical form of the Jacobian for this problem. **[4 marks]**

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Answer:

$\mathbf{U} = (u_1, u_2)^T = (x, y)^T$

[1 mark]

$F_1(\mathbf{U}) = u_1^2 u_2 - 2$
$F_2(\mathbf{U}) = u_1 + u_2^2 - 1$

[1 mark]

$$J = \begin{pmatrix} 2u_1u_2 & u_1^2 \\ 1 & 2u_2 \end{pmatrix}$$

[2 marks]

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(b) Using a single step of Newton's Method compute an approximation to a root of this equation system starting from the point $(x, y) = (1, 1)$. **[4 marks]**

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Answer:

$U = (1, 1)$

$F = (-1, 1)$, $|F| = 2^{1/2}$

[1 mark]

Compute $J = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$

[1 mark]

Solve $J\delta = -F$ for $\delta = (1, -1)$

Update $U = (1, 1) + (1, -1) = (2, 0)$

[1 mark]

$F = (-2, 1)$, $|F| = 5^{1/2}$

[1 mark]

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(c) The standard Newton algorithm can be extended to include a Line Search algorithm.

(i) Describe the purpose of Line Search as part of the overall algorithm.

(ii) State the modification to the Newton algorithm in this case.

(iii) Describe a practical Line Search algorithm that could be used.

(iv) Include a description of the successful and unsuccessful termination of the Line Search algorithm.

[6 marks]

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Answer:

Line search is used to try and prevent Newton's method from diverging [1 mark]

The Newton update step $U = U + \delta$ is modified to a damped form $U = U + \lambda\delta$ [1 mark]

λ is chosen on the range $0 < \lambda \leq 1$ [1 mark]

A Line Search step-halving approach can be used.

The current solution U^k and function norm $|F^k|$ are stored

0. Set $\lambda = 1$, $tries = 0$

1. Evaluate $U^{k+1} = U^k + \lambda\delta$ and $|F^{k+1}| = F(U^{k+1})$ [1 mark]

2. If $|F^{k+1}| < |F^k|$ accept U^{k+1} and return success [1 mark]

3. Set $\lambda = \lambda/2$ and $tries = tries + 1$

4. If $tries > maxTries$ return failure, else goto 1. [1 mark]

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(d) Compute one step of the Newton algorithm including Line Search, starting from the point $(x, y) = (1, 1)$ as before. **[4 marks]**

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Answer:

From (a) $U^k = (1, 1)$, $|F^k| = 2^{1/2}$, $\delta = (1, -1)$

$\lambda = 1$, $U^{k+1} = (2, 0)$, $F^{k+1} = (-2, 1)$, $|F^{k+1}| = 5^{1/2}$ [1 mark]

$|F^{k+1}| > |F^k|$ so set $\lambda = 1/2$ [1 mark]

$U^{k+1} = (1.5, 0.5)$, $F^{k+1} = (-0.825, 0.75)$, $|F^{k+1}| = 1.32$ [1 mark]

$|F^{k+1}| < |F^k|$ so return success [1 mark]

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(e) Explain why combining Newton's Method with the Bisection Method is preferred to Line Search in the case of scalar nonlinear equations. **[2 marks]**

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Answer:

The Bisection Method guarantees convergence of the overall algorithm to a root once a valid bracket is located. [1 mark]

Line Search cannot guarantee convergence of the overall algorithm. [1 mark]

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[question 1 total: 20 marks]

Question 2

A function $u(x,t)$ satisfies the following nonlinear partial differential equation

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(g(u)\frac{\partial u}{\partial x}\right) + u^2, \tag{3}$$

for $x \in [0,1]$ with boundary conditions $u(0,t) = 0$, $u(1,t) = 0$, and $t > 0$ with initial conditions $u(x,0) = U_0(x)$. $g(u)$ is a known, always positive, function of the solution u.

On a uniform grid of m nodes, with nodal spacing h, covering the domain $x \in [0,1]$, we can write a numerical approximation to the PDE (**??**) at a typical internal node i as,

$$\frac{u_i^{k+1} - u_i^k}{\Delta t} = \frac{1}{h^2}\left(g(u_{i+\frac{1}{2}}^{k+1})(u_{i+1}^{k+1} - u_i^{k+1}) - g(u_{i-\frac{1}{2}}^{k+1})(u_i^{k+1} - u_{i-1}^{k+1})\right) + \left(u_i^{k+1}\right)^2 \tag{4}$$

(a) State two alternative, consistent forms for the discretisation of the factor $g(u_{i+\frac{1}{2}}^{k+1})$. **[2 marks]**

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Answer:

(a)

$$g(u_{i+\frac{1}{2}}^{k+1}) = \frac{1}{2}\left(g(u_i^{k+1}) + g(u_{i+1}^{k+1})\right)$$

[1 mark]

$$g(u_{i+\frac{1}{2}}^{k+1}) = g\left(\frac{1}{2}\left(u_i^{k+1} + u_{i+1}^{k+1}\right)\right)$$

[1 mark]

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(b) State the size of the nonlinear system that would be solved in this case, and the precise form of the solution vector $\mathbf{U}$ that would be required. **[2 marks]**

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Answer:

(b)

There are $m-2$ unknown solution values on the grid.

[1 mark]

Assuming we number the grid from 1 to m, $\mathbf{U} = (u_2, u_3, \ldots, u_{m-1})$ is the set of $m-2$ unknown solution values.

[1 mark]

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(c) Describe the algorithm required to advance the model in time. This should include:

- initialisation of the time stepping;
- a suitable initial state for Newton's method at each time step.

[3 marks]

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Answer:

(c)

$t = 0$

Set initial solution U^0 from initial conditions $U_i^0 = U_0(x_i)$

[1 mark]

for k = 0 to maxSteps

$t = t + \Delta t$

Initial guess $U_0^{k+1} = U^k$ [1 mark]

U^{k+1} = Newton(pdeModel, Jacobian, U_0^{k+1}, Tol) [1 mark]

end

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(d) (i) Explain why the Jacobian for this nonlinear system has tridiagonal structure. State the precise number of non-zero entries (nz) as a function of the number of equations in your system N.

(ii) State which steps of the Newton algorithm can be made more efficient, in terms of memory and CPU time, for a problem with a tridiagonal Jacobian. In each case give a reason for your answer.

[7 marks]

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Answer:

(d)(i)

An equation F_i in this system only depends on 3 solution values: $F_i(u_{i-1}, u_i, u_{i+1}) = 0$

[1 mark]

Hence only Jacobian terms J_{ii-1},J_{ii},J_{ii+1} are non-zero and the system is tridiagonal

[1 mark]

There are $3N - 2$ non-zeros in the Jacobian

[1 mark]

(d)(ii)

Computing the Jacobian matrix at each Newton iteration [1 mark]

The Jacobian matrix can be computed analytically, requiring only the non-zero entries to be computed with $\mathcal{O}(N)$ work. The Jacobian can be stored in a sparse matrix structure requiring $\mathcal{O}(N)$ storage [1 mark]

Solving the linear system $J\delta = -f$ at each Newton iteration. [1 mark]

The system can be solved with a tridiagonal solution algorithm (Thomas algorithm) with $\mathcal{O}(N)$ work. [1 mark]

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(e) (i) Describe an efficient numerical approximation to the Jacobian matrix that could be made assuming the tridiagonal sparse structure.

(ii) State one advantage and one disadvantage of an analytical form of the Jacobian in this case.

[6 marks]

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Answer:

(e)(i)

A term of the Jacobian can be approximated numerically by the difference

$$J_{ij} = \frac{\partial F_i}{\partial u_j} = \frac{F_i(\mathbf{u} + \epsilon u_j) - F_i(\mathbf{u})}{\epsilon}$$

[1 mark]

Each column of the Jacobian has only 3 non-zero entries hence we can form 3 non-overlapping sets of Jacobian columns [1 mark]

The numerical approximation can be applied to each set as one function evaluation $F_(\mathbf{u} + \epsilon u_j)$ where u_j varies depending which Jacobian column we are computing. [1 mark]

The columns of the Jacobian can be extracted from the resulting vector in groups of 3. [1 mark]

(e)(ii)

Advantage: The analytical form would be at least as efficient as the numerical approximation and would be numerically exact up to round-off error. [1 mark]

Disadvantage: The analytical Jacobian terms have to calculated in a problem-specific way. [1 mark]

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[question 2 total: 20 marks]

Question 3

A two-dimensional nonlinear PDE for $u(x, y)$ is defined as

$$\frac{\partial}{\partial x}\left(u^4 \frac{\partial u}{\partial x}\right) + \frac{\partial^2 u}{\partial y^2} \;=\; 0 \tag{5}$$

for the spatial domain $(x, y) \in [0, 1] \times [0, 1]$. On the boundary of the domain, boundary conditions $u(x, y) = U_b(x, y)$ are known.

A uniform mesh of m nodes is used in each coordinate direction, with nodal spacing h.

Applying standard finite difference approximations in space a possible discretised form of this problem is given by Equation (**??**).

$$\frac{1}{16h^2}\Big(\left(u_{i+1j} + u_{ij}\right)^4 \left(u_{i+1j} - u_{ij}\right) - \left(u_{ij} + u_{i-1j}\right)^4 \left(u_{ij} - u_{i-1j}\right)\Big) + \frac{1}{h^2}\left(u_{ij+1} - 2u_{ij} + u_{ij-1}\right) \;=\; 0 \tag{6}$$

where $u_{ij} \equiv u(x_i, y_j)$, $i, j = 2, ..., m-1$.

(a) Deduce the sparse structure of the Jacobian matrix for this problem, stating a realistic bound on the number of non-zero entries in the matrix.

[4 marks]

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Answer:

(a)

An equation F_{ij} depends on 5 solution values $F_{ij}(u_{ij-1}, u_{i-1j}, u_{ij}, u_{i+1j}, u_{ij+1})$ [1 mark]

There are $N = (m-2)^2$ equations and a realistic bound is $nz < 5N$ [1 mark]

If a row-by-row numbering system is adopted, the structure of the Jacobian is an $(m-2) \times (n-2)$ array of blocks each of size $(m-2) \times (m-2)$ [1 mark]

The blocks on the diagonal are tridiagonal, neighbouring off-diagonal blocks are diagonal, all other blocks are zero. [1 mark]

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(b) The Jacobian matrix is determined to be numerically symmetric and positive definite.

Assuming the Jacobian can be computed, describe an efficient iterative solution strategy for the linear equations system at each Newton iteration. **[3 marks]**

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Answer:

(b)

The Conjugate Gradient method would be the most appropriate choice [1 mark]

Preconditioning should be used to increase efficiency [1 mark]

For this system an Incomplete Choleski decomposition could be used [1 mark]

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(c) If the discrete system (**??**) is written in the form $\mathbf{F}(\mathbf{U}) = \mathbf{0}$ describe a pseudo-timestepping solution algorithm for this problem.

State one advantage and one disadvantage of this approach. **[6 marks]**

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Answer:

(c) The pseudo-timestepping approach can be used to set up a time dependent nonlinear problem

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{F}(\mathbf{U}) = \mathbf{0}$$

[1 mark]

The given initial guess U_0 becomes the initial conditions for the time stepping [1 mark]

Each time step requires the solution of a nonlinear system, but we have an accurate initial state from the previous time step. [1 mark]

Time steps continue until a steady state is reached, which is the solution of the original nonlinear system [1 mark]

Advantage: Removes problems associated with the initial state for Newton's method [1 mark]

Disadvantage: Requires the solution of a series of nonlinear problems rather than just one. [1 mark]

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(d) How would your answers to parts (a)-(c) change if the three-dimensional form of the PDE (**??**) was to be solved? **[3 marks]**

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Answer:

(d)

The sparsity pattern would change. The overall structure would expand to reflect the 3D finite difference grid. [1 mark]

The matrix would still be SPD and preconditioned CG in the form described in (c) could be used. [1 mark]

The pseudo-timestepping approach (d) would still be valid and work in the same way [1 mark]

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(e) State two advantages and two disadvantages of iterative linear algebra, compared to direct linear algebra for these problems. **[4 marks]**

Answer:

Advantage: Iterative algorithms can produce an acceptable, approximate solution with much less work than solving with a direct algorithm. [1 mark]

Advantage: Iterative methods are straightforward to apply to large, sparse equation systems, direct methods are more complex. [1 mark]

Disadvantage: Iterative linear algebra algorithms require an effective preconditioner to be efficient. [1 mark]

Disadvantage: Direct algorithms guarantee a solution with a known amount of work, iterative methods do not. [1 mark]

[question 3 total: 20 marks]

[grand total: 60 marks]