A14538W1

MASTER OF SCIENCE

Mathematical Modelling and Scientific Computing

Numerical Linear Algebra and Continuous Optimisation

TRINITY TERM 2024

Friday 19th April 2024, 9:30am - 12:00pm

This exam paper contains two sections. You may attempt as many questions as you like but you must answer at least one question in each section. Your best answer in each section will count, along with your next best two answers, making a total of four answers.

Do not turn this page until you are told that you may do so

Numerical Linear Algebra

1. (a) [16 marks] State the pseudo-code to compute both the unitary matrix Q and the unitary similar upper Hessenberg matrix H of a general matrix A such that $A = QHQ^*$. Determine the number of flops, to leading order, required to compute both Q and H.

   (b) [9 marks] Show that, for any matrix $A \in \mathbb{R}^{m\times n}$, there exist unitary matrices U and V such that $A = UBV^T$, where B is nonzero for all entries except B_{ii} for $i = 1, \ldots, \min(m, n)$ and $B_{i+1,i}$ for $i = 1, \ldots, \min(m, n) - 1$.

2. (a) [11 marks] Consider an algorithm of the form $x^{(k+1)} = x^{(k)} + \alpha_k A(b - Ax^{(k)})$ to compute an approximate solution of $Ax = b$ for A hermitian, $A^* = A$. Let $e^{(k)} = x - x^{(k)}$ denote the error at iteration k. How should α_k be defined such that it minimizes $\|e^{(k+1)}\|_2$? Provide a bound on the error of the form

$$\|e^{(k+1)}\|_2 \leqslant \delta \|e^{(k)}\|_2,$$

where δ is a function of the condition number of A.

(b) [5 marks] The k^{th} iterate of GMRES, with $x^{(0)} = 0$, minimizes $\|r^{(k)}\|_2$ over the Kyrlov subpace $b + \text{span}(Ab, A^2b, \cdots, A^{k-1}b) = b + \mathcal{K}_k(b, A)$, namely,

$$x^{(k)} = \text{argmin}_z \|b - Az\|, \quad \text{subject to} \quad z \in \mathcal{K}_k(b, A).$$

By computing $A^j b$ for $j = 0, ..., k-1$ explain why GMRES does not compute the Krylov subspace directly.

(c) [9 marks] The k^{th} iterate of GMRES uses an orthogonal basis, say Q_k, of

$$b + \text{span}(Ab, A^2b, \cdots, A^{k-1}b) = b + \mathcal{K}_k(b, A).$$

Explain a computationally efficient method by which Q_{k+1} can be computed for the next iteration of GMRES.

Continuous Optimisation

3. Consider the following unconstrained optimization problem

$$\min_{x \in \mathbb{R}^n} \; f(x), \tag{1}$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable and bounded below.

(a) [3 marks] Describe the Generic Linesearch Method (GLM) applied to (1).

(b) [6 marks] On each iteration of the GLM, consider using the Armijo condition to calculate a stepsize $\alpha_k > 0$ such that

$$f(x^k + \alpha_k s^k) \leqslant f(x^k) + \beta \alpha_k \nabla f(x^k)^T s^k, \tag{2}$$

where $\beta \in (0, 1)$, x^k is the current iterate and s^k is the step. Show that there exists $\overline{\alpha}_k > 0$ such that (2) is satisfied for all $\alpha \in [0, \overline{\alpha}_k]$.

(c) [5 marks] Describe the backtracking technique that can be used on the kth iteration of the GLM to calculate a stepsize $\alpha_k > 0$ satisfying the Armijo condition given in (2).

Prove an upper bound on the number of backtracking iterations that are needed to satisfy the Armijo condition in (2).

(d) [4 marks] Assume that the gradient $\nabla f(\cdot)$ of f is Lipschitz continuous on $\mathbb{R}^n$. Show that, for any $x \in \mathbb{R}^n$ and $s \in \mathbb{R}^n$,

$$f(x + d) \leqslant f(x) + d^T \nabla f(x) + c \cdot L \cdot \|d\|^2, \tag{3}$$

where L is the Lipschitz constant of the gradient ∇f, $c > 0$ is a constant you should specify, and $\|\cdot\|$ denotes the Euclidean norm.

(e) [7 marks] Apply the steepest descent method with exact linesearch to problem (1). Using (3) for suitable choices of x and d, or otherwise, show that this method is globally convergent, namely, that the gradient at the iterates converges to zero as the number of iterations increase.

4. Consider the unconstrained optimization problem

$$\min_{x \in \mathbb{R}^n} \ f(x), \tag{1}$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is twice continuously differentiable. Let $\nabla f(\cdot)$ and $\nabla^2 f(\cdot)$ denote the gradient and the matrix of second-derivatives (ie, the Hessian) of f, respectively.

(a) [5 marks] Let x^* be a stationary point of f. Apply Newton's method for optimization to (1), without linesearch. State the conditions required on f and its derivatives, as well as on some Newton iterate, such that Newton's method converges, with quadratic rate, to x^*.

(b) [6 marks] Consider the following function

$$f(x) = x_1^m + 2x_2^p + 3x_3^q, \tag{2}$$

where $x = (x_1, x_2, x_3)^T \in \mathbb{R}^3$, and $m \geqslant 2$, $p \geqslant 2$ and $q \geqslant 2$ are natural numbers. Apply Newton's method (without linesearch) to minimizing f, starting at $x^0 \in \mathbb{R}^3$, where $x_i^0 \neq 0$ for all $i \in \{1, 2, 3\}$.
Calculate the Newton iterates, and establish their convergence and rate of convergence.
Explain why this convergence rate is not quadratic.
Find the values of m, p and q that give the fastest convergence.

(c) Assume that the function f in (1) is a least squares, namely,

$$\min_{x \in \mathbb{R}^n} f(x) = \frac{1}{2}\|r(x)\|^2, \tag{3}$$

where $r : \mathbb{R}^n \to \mathbb{R}^m$ is twice-continuously differentiable with $m \geqslant n$ and $\|\cdot\|$ denotes the Euclidean norm.

(i) [8 marks] Write down an expression for the gradient $\nabla f(x)$ and the Hessian matrix $\nabla^2 f(x)$ of f in (3) as a function of the residual $r(x)$ and its derivatives.

Using these, and an approach using linear least squares, present two ways to derive the expression of the Gauss-Newton search direction s_{GN}^k from a point x^k for (3).

Give a condition on the Jacobian of r at x^k such that s_{GN}^k is a descent direction for f; justify your answer.

(ii) [6 marks] State a theorem of global convergence for the Gauss-Newton method with backtracking Armijo linesearch. *[Hint: There is no need to state/define the backtracking-Armijo linesearch as part of the theorem statement.]*

5. (a) [12 marks] Consider the function

$$h(x) = -\frac{1}{2}x_1^2 + \frac{1}{2}x_1 x_2^2 + \frac{8}{3}x_1^6, \tag{1}$$

where $x = (x_1\ x_2)^T \in \mathbb{R}^2$.

(i) Find all stationary points of the function $h(x)$ for $x \in \mathbb{R}^2$.

(ii) Investigate the nature of each of the stationary points, namely, establish whether they are local minimizers, maximizers or saddle points.

(iii) Does $h(x)$ have any global minima or maxima? Justify your answer.

(b) [13 marks] Consider the equality-constrained optimization problem,

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad c(x) = 0, \tag{2}$$

where $f : \mathbb{R}^n \to \mathbb{R}$ and $c : \mathbb{R}^n \to \mathbb{R}^m$ with $c(x) = (c_1(x), \dots, c_m(x))^T$ are continuously differentiable functions, and $m \leqslant n$.

(i) Assuming a suitable constraint qualification holds (that you do not need to define), show that any local minimizer of (2) is a KKT point of (2).

(ii) Briefly describe the role of the constraint qualification in this proof and give one example of a suitable constraint qualification for problem (2).

6. (a) [7 marks] Assume that D is a diagonal and positive-definite $n \times n$ matrix. We define the D-norm of a vector s such that $\|s\|_D^2 = s^T D s$. Find necessary and sufficient conditions for s^* to be a global minimiser of the problem,

$$\min_{s \in \mathbb{R}^n} m(s) = s^T g + \frac{1}{2} s^T H s \text{ subject to } \|s\|_D \leqslant \Delta, \tag{1}$$

where $\Delta > 0$, $g \in \mathbb{R}^n$ and H is a real symmetric $n \times n$ matrix; and $a^T b$ represents the Euclidean inner product of two vectors a and b in $\mathbb{R}^n$.

(b) Consider the equality-constrained optimization problem,

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{subject to} \quad c(x) = 0, \tag{2}$$

where $f : \mathbb{R}^n \to \mathbb{R}$ and $c : \mathbb{R}^n \to \mathbb{R}^m$ with $c(x) = (c_1(x), \ldots, c_m(x))^T$ are continuously differentiable functions.

(i) [3 marks] Describe the connections between the local minimizers of problem (2) and the local minimizers of the quadratic penalty function associated with (2).

(ii) [6 marks] State the theorem of global convergence for the quadratic penalty method applied to problem (2). Prove that the iterates x^k of this method are asymptotically feasible for problem (2) as $k \to \infty$. [*Hint: in your proof, you may assume that the Lagrange multiplier estimates y^k converge to the optimal Lagrange multiplier y^* of the constraints.*]

(iii) [5 marks] Assume that on each major iteration of the quadratic penalty method, a generic trust region method is employed to minimize the corresponding quadratic penalty function. State (without proof) conditions under which this (inner) minimization can be terminated successfully, irrespective of the starting point.

(iv) [4 marks] In the conditions of part (b)(iii), assume that the (usual) trust region constraint in the inner minimization is scaled by a matrix D as in (1) that is allowed to change iteratively. In the context of quadratic penalty method, describe the potential advantages of using (1), instead of the usual formulation of the trust-region constraint, and propose a suitable choice of D in this case.