A14538W1

DEGREE OF MASTER OF SCIENCE

Mathematical Modelling and Scientific Computing

Numerical Linear Algebra and Continuous Optimisation

Trinity Term 2023

Friday, 21 April 2023, 2:30pm to 5.00pm

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.

Candidates may bring a summary sheet into this exam consisting of (both sides of) one sheet of A4 paper containing material prepared in advance in accordance with the guidance given by the Mathematical Institute.

Please start the answer to each question in a new booklet.

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

Numerical Linear Algebra

1. (a) [14 marks] Let $A \in \mathbb{R}^{n\times n}$, and let p be a polynomial $p(z) = \sum_{i=0}^{k} c_i z^i$. Consider $p(A) = \sum_{i=0}^{k} c_i A^i$.

   (i) Let $\{\lambda_i\}_{i=1}^{n}$ denote the eigenvalues of $A \in \mathbb{R}^{n\times n}$. Find the eigenvalues of A^2, and those of $p(A)$.

   (ii) Suppose that A is normal, and q is another polynomial such that $|p(z) - q(z)| \leqslant \epsilon$ for all $z \in \{\lambda_1, \ldots, \lambda_n\}$. Prove that

$$\|p(A) - q(A)\|_2 \leqslant \epsilon.$$

   [*Recall that a normal matrix A has an eigenvalue decomposition $A = Q\Lambda Q^*$, where $\Lambda = diag(\lambda_i)$ and Q is unitary.*]

   (iii) Drop the assumption that A is normal in (ii), but suppose A is diagonalisable, $A = X\Lambda X^{-1}$. Give an upper bound for $\|p(A) - q(A)\|_2$ involving ϵ and $\kappa_2(X) = \|X\|_2\|X^{-1}\|_2$.

   (iv) Suppose that A is normal, and the eigenvalues of A lie in a disk of radius 1, centered at 2. Prove that there exists a polynomial p of degree k such that $p(0) = 1$ and

$$\|p(A)\|_2 \leqslant 2^{-k}. \tag{1}$$

   (b) [11 marks] Consider the GMRES algorithm for solving a linear system $Ax = b$ where $b \in \mathbb{R}^n$. Recall that after k iterations, GMRES finds the solution x_k in the Krylov subspace $\mathrm{Span}[b, Ab, \ldots, A^{k-1}b]$ that minimises the residual $\|Ax_k - b\|_2$.

   (i) Suppose that one obtains the Arnoldi decomposition $AQ_k = Q_{k+1}\tilde{H}_k$ where $Q_k = [q_1, \ldots, q_k]$, $Q_{k+1} = [q_1, \ldots, q_{k+1}]$ are orthonormal with $q_1 = b/\|b\|_2$, and $\tilde{H}_k \in \mathbb{R}^{(k+1)\times k}$ is upper Hessenberg with nonzero subdiagonal entries $(\tilde{H}_k)_{i+1,i} \neq 0$ for all i. Prove that $\mathrm{Span}[q_1, \ldots, q_\ell] = \mathrm{Span}[b, Ab, \ldots, A^{\ell-1}b]$, for $\ell = 1, 2, \ldots, k$.

   (ii) Express $H_k \in \mathbb{R}^{k\times k}$, the upper $k \times k$ part of $\tilde{H}_k$, using Q_k and A.

   (iii) In the setting of (a)-(iv), show that the GMRES solution x_k after k steps satisfies $\|Ax_k - b\|_2 \leqslant 2^{-k}\|b\|_2$.

2. Consider the least-squares problem

$$\min_x \|Ax - b\|_2, \tag{1}$$

where $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$ with $m \gg n$. Also let $S \in \mathbb{R}^{s \times m}$ $(s > n)$ and consider

$$\min_y \|SAy - Sb\|_2. \tag{2}$$

Assume that $\operatorname{rank}(A) = \operatorname{rank}(SA) = n$. Let x_* denote the solution for (1), and y_* the solution for (2).

(a) [8 marks] (i) Express x_* and y_* in terms of A, b, and S.

(ii) Given A, SA, b, and Sb, find the computational complexity of solving (1) and (2) using a classical QR-based method in the big-O notation, e.g. $O(sn), O(m^2ns)$.

(b) [17 marks] Let $[A, b] = QR$ be a QR factorisation, where $Q \in \mathbb{R}^{m \times (n+1)}$ and $R \in \mathbb{R}^{(n+1)\times(n+1)}$.

(i) Show that for any vector $v \in \mathbb{R}^{n+1}$, we have

$$\sigma_{n+1}(SQ)\|Rv\|_2 \leqslant \|S[A, b]v\|_2 \leqslant \sigma_1(SQ)\|Rv\|_2,$$

where $\sigma_i(SQ)$ denotes the ith largest singular value of SQ.
[*You may use the fact* $\sigma_{n+1}(B) \leqslant \|Bx\|_2/\|x\|_2 \leqslant \sigma_1(B)$ *for any* $B \in \mathbb{R}^{s\times(n+1)}$, *and any vector* x *(this is a special case of the Courant-Fischer theorem).*]

(ii) By choosing a particular v in (i), prove that

$$\|S(Ax_* - b)\|_2 \leqslant \sigma_1(SQ)\|Ax_* - b\|_2.$$

Similarly, prove that

$$\|S(Ay_* - b)\|_2 \geqslant \sigma_{n+1}(SQ)\|Ay_* - b\|_2.$$

(iii) Using the above results, or otherwise, prove that

$$\|Ax_* - b\|_2 \leqslant \|Ay_* - b\|_2 \leqslant \kappa_2(SQ)\|Ax_* - b\|_2.$$

Continuous Optimisation

3. Consider the unconstrained optimisation problem

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

where $f:\mathbb{R}^n \to \mathbb{R}$ is continuously differentiable with gradient ∇f, which is Lipschitz continuous so that $\|\nabla f(x) - \nabla f(y)\| \leqslant L\|x-y\|$ for all $x, y \in \mathbb{R}^n$. Assume f is bounded from below. To solve (1) we consider using a Generic Linesearch Method (GLM) with initial guess $x^0 \in \mathbb{R}^n$. Let s^k be the search direction, and α^k the stepsize, so that the iterates are $x^{k+1} = x^k + \alpha^k s^k$.

(a) [15 marks] Consider using backtracking Armijo linesearch, with backtracking parameter $\tau \in (0,1)$ and initial stepsize $\alpha_{(0)}$, and finding a stepsize such that the Armijo condition $f(x^k + \alpha^k s^k) \leqslant f(x^k) + \beta\alpha^k \nabla f(x^k)^T s^k$ is satisfied. Below, assume $\alpha_{(0)}$ is suficiently large.

(i) Show that the stepsize α^k is bounded from below by $\tau(1-\beta)\frac{|\nabla f(x^k)^T s^k|}{L\|s^k\|^2}$.

(ii) Let θ^k be the angle between $-\nabla f(x^k)$ and s^k, that is, $\cos\theta^k = \frac{-\nabla f(x^k)^T s^k}{\|\nabla f(x^k)\|\|s^k\|}$. Using (i), or otherwise, show that for any $\epsilon > 0$, there exists a k such that $\|\nabla f(x^k)\|\|s^k\|\cos\theta^k \leqslant \epsilon$.

(iii) Is (ii) enough to establish global convergence of GLM to a stationary point, that is, $\|\nabla f(x^{\tilde{k}})\| < \epsilon$ for some $\tilde{k}$?

(iv) Show that when $s^k = -\nabla f(x^k)$, GLM converges globally to a stationary point.

(b) [10 marks] Consider the use of exact linesearch in GLM.

(i) When $f(x)$ is a quadratic function $f(x) = g^T x + \frac{1}{2}x^T H x$ with $H \succ 0$, find the stepsize α^k with exact linesearch that minimises $f(x^k + \alpha^k s^k)$, given x^k and s^k.

(ii) Consider taking s^k to be a random vector (e.g. Gaussian vector with iid $N(0,1)$ entries). In each iteration, we attempt a number of such random search directions with exact linesearch, and adopt the one with the lowest objective function value. Briefly discuss if this is an efficient algorithm in high-dimensional problems $n \gg 1$, referring to the results in (a).

(iii) Show that with exact linesearch we have $\nabla f(x^{k+1})^T s^k = 0$, that is, the gradient in the next step is orthogonal to the previous search direction.

4. Consider the unconstrained problem minimise$_x$ $f(x)$, where $f : \mathbb{R}^n \to \mathbb{R}$ is twice continuously differentiable.

   (a) [15 marks] Let $A \in \mathbb{R}^{n\times n}$ be a nonsingular matrix and define $\bar{f}(y) = f(A^{-1}y)$.

   (i) Find the gradient of $\bar{f}$ with respect to y, that is, $\nabla \bar{f} = \left[\frac{\partial \bar{f}}{\partial y_1}, \frac{\partial \bar{f}}{\partial y_2}, \ldots, \frac{\partial \bar{f}}{\partial y_n}\right]^T$.

   (ii) Show that $\nabla^2 \bar{f} = A^{-T} H A^{-1}$, where $H = \nabla^2 f$.

   (iii) Suppose that H is positive definite. Find a matrix A such that $\nabla^2 \bar{f} = I$.

   (iv) Suppose that f is a convex quadratic $f(x) = g^T x + \frac{1}{2} x^T H x$ with $H \succ 0$. Find the first iterate x^1 with $x^0 = 0$ when the steepest descent method with exact linesearch is applied to minimise$_y$ $\bar{f}(y)$, with the choice of A in (iii).

   (b) [10 marks] Recall that the quasi-Newton method approximates $\nabla^2 f(x^k)$ by a symmetric matrix B^k that satisfies the secant equation $B^{k+1}(x^{k+1} - x^k) = \nabla f(x^{k+1}) - \nabla f(x^k)$.

   (i) Suppose that B^k is positive definite. Show that $-(B^k)^{-1}\nabla f(x^k)$ is a descent direction.

   (ii) In most quasi-Newton methods B^k is updated with a low-rank matrix. Briefly explain the computational advantages of doing so.
   [*You may want to refer to the Sherman-Morrison-Woodbury formula, but you need not write down the precise formula.*]

   (iii) Consider using a rank-two update $B^{k+1} = B^k + \alpha u u^T + \beta v v^T$, where $\alpha, \beta \in \mathbb{R}$ and $u, v \in \mathbb{R}^n$. Define $\delta = x^{k+1} - x^k$ and $\gamma = \nabla f(x^{k+1}) - \nabla f(x^k)$, so that the secant equation can be written as $B^{k+1}\delta = \gamma$. By choosing $u = B^k\delta$ and $v = \gamma$, derive the update formula for B^k (i.e., find α and β) in the BFGS quasi-Newton method.
   [*You may assume that $B^k\delta$ and γ are linearly independent.*]

5. Consider the constrained convex optimisation problem

$$\min_{x\in\mathbb{R}^n} f(x) \quad \text{subject to} \quad c(x) \geqslant 0 \quad \text{and} \quad Ax = b, \tag{1}$$

where $f : \mathbb{R}^n \to \mathbb{R}$ and $c = [c_1, c_2, \ldots, c_p]^T : \mathbb{R}^n \to \mathbb{R}^p$ are continuously differentiable, f is convex, each c_i is concave (i.e., $-c_i$ is convex), and $A \in \mathbb{R}^{m\times n}$ with $m \leqslant n$ and $b \in \mathbb{R}^m$.

[*Recall that f is convex if $f(\alpha x + (1-\alpha)y) \leqslant \alpha f(x) + (1-\alpha) f(y)$ for all x, y and $\alpha \in (0,1)$. As f is differentiable, we also have $f(y) - f(x) \geqslant \nabla f(x)^T(y-x)$ for all $x, y \in \mathbb{R}^n$.*]

(a) [15 marks] (i) Suppose that $\nabla f(\tilde{x}) = 0$. Show that $\tilde{x}$ is the minimiser of the unconstrained problem $\min_{x\in\mathbb{R}^n} f(x)$.

(ii) Show that the feasible set Ω of (1) is convex.
[*A set Ω is convex if for any $x, y \in \Omega$ and $\alpha \in [0,1]$, $\alpha x + (1-\alpha)y \in \Omega$.*]

(iii) Suppose that (x^*, y, λ) satisfy the KKT conditions for the convex problem (1). Prove that for any feasible $x \in \Omega$,

$$f(x) \geqslant f(x^*) + \sum_{i=1}^{p} \lambda_i \nabla c_i(x^*)^T (x - x^*).$$

[*Recall that the KKT conditions for* (1) *are:* $\nabla f(x^*) = A^T y + \sum_{i=1}^{p} \lambda_i \nabla c_i(x^*)$, *where* $\lambda = [\lambda_1, \lambda_2, \ldots, \lambda_p]^T$ *with* $\lambda_i \geqslant 0$, $\lambda_i c_i(x^*) = 0$ *for all* i, *and* $x^* \in \Omega$.]

(iv) Using (iii), or otherwise, show that x^* is a global minimiser of (1).

(b) [10 marks] Consider the Lagrangian $\mathcal{L} : \mathbb{R}^{n+m+p} \to \mathbb{R}$

$$\mathcal{L}(x, y, \lambda) := f(x) - y^T(Ax - b) - \sum_{i=1}^{p} \lambda_i c_i(x),$$

and define $g(y, \lambda) := \min_x \mathcal{L}(x, y, \lambda)$.

(i) Show that for any fixed (y, λ) where $\lambda \geqslant 0$, we have $g(y, \lambda) \leqslant f(x^*)$, where x^* is the global minimiser of (1). Is the convexity of f and c_i needed for this result?

(ii) Assuming that x^* satisfies the KKT conditions for (1), prove that

$$\max_{y, \lambda \geqslant 0} g(y, \lambda) = f(x^*).$$

6. Consider the trust-region subproblem (TRS)

$$\underset{s}{\text{minimise}}\ m(s) = g^T s + \frac{1}{2} s^T H s, \qquad \text{subject to} \quad \|s\| \leqslant \Delta. \tag{1}$$

Here $H \in \mathbb{R}^{n\times n}$ is symmetric, and $g \in \mathbb{R}^n$.

(a) [12 marks] Recall that the KKT conditions for the TRS are: there exists $\lambda^* \geqslant 0$ such that

$$\begin{aligned} (H + \lambda^* I)s &= -g, \\ \lambda^*(\|s\| - \Delta) &= 0, \\ \|s\| &\leqslant \Delta. \end{aligned} \tag{2}$$

Recall also that the global solution for the TRS satisfies $(H + \lambda^* I) \succeq 0$ in addition to the KKT conditions.

(i) Briefly explain how the TRS arises in the context of a trust-region method for minimising $f(x)$, where $f : \mathbb{R}^n \to \mathbb{R}$ is twice continuously differentiable.

(ii) Suppose the TRS solution s^* satisfies $\|s^*\| < \Delta$. Prove that $H \succeq 0$, and find an expression for s^* when $H \succ 0$.

(iii) Let $\hat{s}(\lambda) = -(H + \lambda I)^{-1} g$. By examining the function $\|\hat{s}(\lambda)\|^2$, or otherwise, show that there is at most one value of λ^* for which the KKT conditions hold together with $H + \lambda^* I \succeq 0$.

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

$$\underset{x\in\mathbb{R}^n}{\text{minimise}}\ f(x), \quad \text{subject to} \quad c(x) = 0, \tag{3}$$

where $f : \mathbb{R}^n \to \mathbb{R}$ and $c : \mathbb{R}^n \to \mathbb{R}^m$ with $c(x) = (c_1(x), \ldots, c_m(x))^T$ $(m \leqslant n)$ are continuously differentiable. Consider the quadratic penalty method that approximately minimises $\Phi_{\sigma^k}(x) = f(x) - \frac{1}{2\sigma^k}\|c(x)\|^2$, for $\sigma^k > 0$, $k \geqslant 0$ at the kth iteration, where $\sigma^k \to 0$.

(i) Suppose that $J(x^k)$ has full $\text{rank}(J(x^k)) = m$. Assuming $\frac{\|c(x^k)\|}{\sigma^k}$ remains bounded, show that $\nabla^2_{xx}\Phi_\sigma(x)$ has m eigenvalues that tend to ∞ as $k \to \infty$.
[*You may use the fact that* $\nabla^2_{xx}\Phi_\sigma(x) = \nabla^2 f(x) + \frac{1}{\sigma}\sum_{i=1}^m c_i(x)\nabla^2 c_i(x) + \frac{1}{\sigma}J(x)^T J(x)$.]

(ii) Comment briefly on the practical drawbacks of the quadratic penalty method as $\sigma^k \to 0$, along with how the augmented Lagrangian method overcomes it.
[*Recall that the augmented Lagrangian method works with the function* $\tilde{\Phi}(x, u, \sigma) = \Phi_\sigma(x) - u^T c(x)$.]

(iii) Assume that $x^k \to x^*$, a KKT point of (3). Find an estimate for the Lagrange multiplier λ using x^k, f, σ^k, and c. Do the same (using also u) when the augmented Lagrangian method is used.