DEGREE OF MASTER OF SCIENCE

MATHEMATICAL MODELLING AND SCIENTIFIC COMPUTING

B2 Further Numerical Linear Algebra and Continuous Optimisation

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TRINITY TERM 2019

FRIDAY, 26 April 2019, 9.30am to 12.00pm

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 answer(s), making a total of four answers.

Please start the answer to each question in a new answer booklet.
All questions will carry equal marks.

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

Section A: Further Numerical Linear Algebra

1. Let Π_k denote the set of real polynomials of degree k or less.

   (a) [5 marks] Let $Ax = b$ be a system of linear equations with $A = M - N$, where M is invertible. If $\{x_k\}$ are iterates generated by a simple iteration

   $$Mx_k = Nx_{k-1} + b, \quad k \geqslant 1,$$

   show how a sequence $\{y_k\}$ can be computed from $\{x_k\}$ such that

   $$x - y_k = p_k(M^{-1}N)\,(x - x_0), \quad p_k \in \Pi_k \text{ with } p_k(1) = 1.$$

   (b) [4 marks] For the situation as described in part (a), if $M = I$,

   $$A = \begin{bmatrix} 3 & 1 & 1 \\ 1 & 3 & 1 \\ 1 & 1 & 3 \end{bmatrix}, \quad b = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, x_0 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix},$$

   and $p_1(z) = -1 + 2z, p_2(z) = 2 - z^2$, calculate y_1 and y_2.

   (c) [6 marks] For the situation as described in part (a), what is the advantage of choosing p_k to be a suitably shifted and scaled Chebyshev polynomial when $M^{-1}N$ is symmetric? You should quote but need not prove any property of the Chebyshev polynomials that you refer to.

   (d) [10 marks] The *Conjugate Gradient* method is an applicable method for the iterative solution of the linear system $Ax = b$ when A is real, symmetric and positive definite. Describe how an *incomplete Cholesky factorization* can be computed for A. How can the triangular incomplete factors be employed in a symmetric *preconditioned* linear system, the solution of which can yield the solution x of the original linear problem. What is the general purpose of employing such a *preconditioner*?

2. (a) [4 marks] Suppose that $B \in \mathbb{R}^{n \times n}$ is a general non-singular matrix. Arnoldi's method applied to B generates a set of orthonormal vectors $\{v_1, v_2, \ldots, v_k\}$ which are the columns of the matrix V_k satisfying

$$BV_k = V_{k+1}\widehat{H}_k.$$

What is the structure of the matrix $\widehat{H}_k$? For what space does $\{v_1, v_2, \ldots, v_k\}$ form an orthonormal basis?

(b) [8 marks] What iterative method for a linear system $Bx = c$ is based on the use of Arnoldi's method and computes iterates x_k for which $\|c - Bx_k\|_2$ is minimal? Give a brief outline of the algorithm for this iterative method.

(c) [6 marks] Suppose that $A \in \mathbb{R}^{m \times m}$ is a real symmetric matrix. How is the algorithmic approach in (a), (b) above modified to give a more efficient algorithm for solving $Ay = b$ with minimal $\|r_k\|_2$ where $r_k = b - Ay_k$ with $\{y_k\}$ being the iterates? For this modified algorithm prove that

$$\|r_k\|_2 \leqslant \min_{p \in \Pi_k, p(0)=1} \max_j |p(\lambda_j)| \, \|r_0\|_2. \qquad (\dagger)$$

where λ_j are the eigenvalues of A. If all of the eigenvalues of A are either -1 or 2, sketch the polynomial $p \in \Pi_2$ which will give the bound for $\|r_2\|_2$ in $(\dagger)$.

(d) [2 marks] A different strategy for finding the solution of the linear system $Bx = c$ as in (b) above using only an iterative method for symmetric matrices is to consider the symmetric matrix

$$A = \begin{bmatrix} 0 & B^T \\ B & 0 \end{bmatrix} \in \mathbb{R}^{2n \times 2n}. \qquad (\star)$$

How can $b \in \mathbb{R}^{2n}$ be chosen so that the solution $x \in \mathbb{R}^n$ to $Bx = c$ can be simply identified from the vector $y \in \mathbb{R}^{2n}$ that satisfies $Ay = b$ where A is defined in $(\star)$?

(e) [5 marks] You are given that all of the $2n$ eigenvalues of the matrix A in $(\star)$ are $\pm\sigma_i, i = 1, \ldots, n$ where $\sigma_i, i = 1, \ldots, n$ are the singular values of B. By considering firstly the convergence bound $(\dagger)$ for $k = 0, 1$ and generalising for larger values of k, deduce that the reduction of $\|r_k\|_2$ with increasing k may occur only on alternate iterations.

Section B: Continuous Optimization

3. (a) [7 marks] 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. State and prove the second-order necessary optimality conditions that hold at a local minimizer x^* of f.

(b) [5 marks] Let f in (1) be defined as

$$f(x_1, x_2) = x_1^4 - a x_2^2 - x_2, \tag{2}$$

where $a > 0$ is a fixed parameter. Show there is only one stationary point of the function (2) and establish whether it is a local minimizer, maximizer or saddle point.

(c) [6 marks] Consider adding inequality constraints to problem (1), yielding the problem

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

where $c : \mathbb{R}^n \to \mathbb{R}^m$ is twice continuously differentiable. Assuming a suitable constraint qualification, state (without proof) the KKT conditions and the second-order necessary optimality conditions that hold at a constrained local minimizer of (3).

(d) [7 marks] Consider problem (3) with f defined in (2) and c (with $m = 1$) defined as

$$c(x_1, x_2) = -x_1^2 - x_2^2 - \frac{2}{a} x_2.$$

Find all the KKT points of problem (3) in this case. For each of the points, using second-order optimality conditions, or otherwise, establish whether they are a minimizer for the given problem.

4. Consider the unconstrained optimization problem

$$\min_{x \in \mathbb{R}^n} f(x), \tag{4}$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable and has a Lipschitz continuous gradient ∇f with Lipschitz constant $L > 0$. Apply the steepest-descent method with linesearch to (4), starting from $x^0 \in \mathbb{R}^n$, where the stepsize is set to $\alpha^k = \overline{\alpha}$ in each iteration $k \geqslant 0$, for some $\overline{\alpha} > 0$ independent of k. We refer to this method as SD-c.

(a) [10 marks] Write down the expression of the new iterate x^{k+1} obtained from x^k using the SD-c algorithm, where $k \geqslant 0$.

Find the optimal value of $\overline{\alpha}$ that guarantees the bound on the function decrease in each SD-c iteration,

$$f(x^k) - f(x^{k+1}) \geqslant \frac{1}{2L}\|\nabla f(x^k)\|^2, \quad k \geqslant 0. \tag{5}$$

[Hint: you may apply (without proof) the following property of functions with Lipschitz continuous gradient, namely,

$$f(x+y) \leqslant f(x) + \nabla f(x)^T y + \frac{L}{2}\|y\|^2, \quad \textit{for any } x \textit{ and } y \in \mathbb{R}^n.]$$

Find minimal conditions on f and $\overline{\alpha}$ such that the SD-c method is globally convergent.

Briefly describe one advantage and one disadvantage of the SD-c method compared to the steepest descent method with backtracking Armijo linesearch studied in the lectures.

(b) Let f in (4) be defined by

$$f(x) = \frac{1}{2}(ax_1^2 + bx_2^2), \tag{6}$$

where $x = (x_1\ x_2)^T \in \mathbb{R}^2$, a and b are given, and $a > b > 0$. Let SD-c method be applied to (6) starting from $x^0 = (1\ 1)^T$.

(i) [4 marks] Show that the iterates x^k, $k \geqslant 0$, generated by the SD-c method satisfy

$$x^k = \Big((1-\overline{\alpha}a)^k \quad (1-\overline{\alpha}b)^k\Big)^T. \tag{7}$$

(ii) [2 marks] Calculate an explicit expression for the optimal value of $\overline{\alpha}$ you found in (a) that ensures the bound (5).

(iii) [9 marks] Show that with the stepsize $\overline{\alpha}$ you calculated in (b)(ii), $\{x^k\}$ converges to the minimizer x^* of f; find the convergence rate and convergence factor.

Relate the factor you found to the one in the local convergence theorem for steepest descent with exact linesearch.

Briefly mention the potential difficulty that the convergence factor may cause and a way to overcome it.

5. Consider

$$\min_{x \in \mathbb{R}^n} f(x), \tag{8}$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable, and let $\nabla f(\cdot)$ denote the gradient of f. Apply a generic trust-region method to (8), where at the kth iterate x^k, the step s^k is calculated by solving (exactly or approximately) the following trust-region subproblem

$$\min_{s \in \mathbb{R}^n} m_k(s) := f(x^k) + s^T \nabla f(x^k) + \frac{1}{2} s^T B^k s \quad \text{subject to} \quad \|s\| \leqslant \Delta_k, \tag{9}$$

where B^k is an $n \times n$ symmetric matrix and $\Delta_k \geqslant 0$ is the trust-region radius.

(a) [8 marks] State a theorem of global convergence for the generic trust-region method with subproblem (9); all assumptions (on f, the value of the model $m_k(s^k)$ and the matrices B^k) should be stated explicitly.
Briefly give one reason for which the theorem you stated is more general than the corresponding convergence result for generic linesearch methods with Newton-like search directions involving B^k (no need to state the latter theorem).

(b) [6 marks] Prove the theorem you stated in (a); you may assume that for all $k \geqslant 0$,

$$f(x^k) - m_k(s^k) \geqslant \frac{1}{2} \|\nabla f(x^k)\| \min \left\{ \Delta_k, \frac{\|\nabla f(x^k)\|}{1 + \|B^k\|} \right\},$$

and there exists a constant $\kappa_d > 0$ independent of k such that $\Delta_k \geqslant \kappa_d \inf_{0 \leqslant i \leqslant k} \|\nabla f(x^i)\|$.

(c) [5 marks] Assume that the symmetric matrix B^k in (9) is updated by a quasi-Newton formula. Namely, after calculating a successful step s^k, we set

$$B^{k+1} = B^k + \beta u v^T,$$

for some $\beta \in \mathbb{R}$ and $u, v \in \mathbb{R}^n$. Using that B^{k+1} must be symmetric and satisfies the secant condition $B^{k+1} s^k = \nabla f(x^{k+1}) - \nabla f(x^k) := \gamma^k$, show that

$$B^{k+1} = B^k + \frac{(\gamma^k - B^k s^k)(\gamma^k - B^k s^k)^T}{(\gamma^k - B^k s^k)^T s^k}. \tag{10}$$

(The expression of B^{k+1} is the so-called symmetric rank-one formula.)

(d) [6 marks] Let $f(x) = \frac{1}{2} x^T x$, where $x \in \mathbb{R}^2$ in (c). If $B^0 = I$ is the 2×2 identity matrix, and assuming that $k = 0$ is a successful iteration, can B^1 be defined by (10)? If $B^0 = \alpha I$ for some $\alpha > 0$, $\alpha \neq 1$ do you foresee any difficulties that may occur when using B^1 defined by (10) in the second iteration of the generic trust-region method?

6. (a) Consider the equality-constrained optimization problem,

$$\min_{x\in\mathbb{R}^2} f(x) := \frac{1}{2}x_1^2 + x_2^2 - 2x_2 \quad \text{subject to} \quad c(x) := x_1 + 4x_2 - 1 = 0, \tag{11}$$

where $x = (x_1\ x_2)^T$. [*Hint: you may assume (without proof) that the solution of problem* (11) *is* $x^* = \left(-\frac{1}{3}\ \frac{1}{3}\right)^T$ *with optimal Lagrange multiplier* $u^* = -\frac{1}{3}$.]

(i) [5 marks] Calculate the global minimizer(s) $x(u,\sigma)$ of the augmented Lagrangian function $\Phi(x,u,\sigma)$ associated with (11), namely, $\Phi(x,u,\sigma) := f(x) - uc(x) + \frac{1}{2\sigma}(c(x))^2$, for $u \in \mathbb{R}$ and $\sigma > 0$.

(ii) [4 marks] Let u be fixed. Show that $x(u,\sigma)$ converges to the solution x^* of problem (11), as $\sigma \to 0$. Let $\nabla^2_{xx}\Phi(x(u,\sigma),u,\sigma)$ denote the matrix of second derivatives (i.e., the Hessian) of $\Phi(\cdot,u,\sigma)$ at $x(u,\sigma)$. Show that the condition number of the matrix $\nabla^2_{xx}\Phi(x(u,\sigma),u,\sigma)$ grows unboundedly, as $\sigma \to 0$.

(iii) [5 marks] Let $\sigma > 0$ be fixed. Let u be updated by the formula

$$u^{k+1} = u^k - \frac{c(x(u^k,\sigma))}{\sigma}, \quad k \geqslant 0, \tag{12}$$

starting from some u^0, and where $x(u^k,\sigma)$ is, like above, the minimizer of $\Phi(x,u^k,\sigma)$. Show that $u^k \to -1/3$ linearly, and that $x(u^k,\sigma) \to x^*$, as $k \to \infty$.

(b) Consider the equality-constrained optimization problem,

$$\min_{x\in\mathbb{R}^n} f(x) \quad \text{subject to} \quad c(x) = 0, \tag{13}$$

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 twice continuously differentiable functions and $m \leqslant n$.

(i) [3 marks] Describe the connection between the stationary points of the quadratic penalty function associated with (13) and a KKT solution of problem (13).

(ii) [6 marks] State the theorem of global convergence for the quadratic penalty method. Prove that the iterates x^k of this method are asymptotically feasible for problem (13) as $k \to \infty$. [*Hint: in your proof, you may assume that the Lagrange multiplier estimates* u^k *converge to the optimal Lagrange multiplier* u^* *of the constraints.*]

(iii) [2 marks] Briefly comment on the quadratic penalty method's disadvantages in connection to the advantages of the augmented Lagrangian's method.