

BSc, MSci and MSc EXAMINATIONS (MATHEMATICS)

May – June 2011

This paper is also taken for the relevant examination for the Associateship of the
Royal College of Science.

Optimisation

Date: Monday, 16 May 2011. Time: 2.00pm. Time allowed: 2 hours.

This paper has FOUR questions.

Candidates should use ONE main answer book.

Supplementary books may only be used after the main book is full.

Statistical tables will not be provided.

- DO NOT OPEN THIS PAPER UNTIL THE INVIGILATOR TELLS YOU TO.
- Answer all the questions. Each question carries equal weight.
- Credit will be given for all questions attempted, but extra credit will be given for complete or nearly complete answers.
- Affix one of the labels provided to each answer book that you use, but DO NOT USE THE LABEL WITH YOUR NAME ON IT.
- Calculators may not be used.

1. Let $f : \mathbb{R}^n \mapsto \mathbb{R}$ be a smooth function and consider Newton's method to minimise f .

- (a) Explain carefully the underlying strategy for obtaining the next iterate \mathbf{x}_{i+1} from the current iterate \mathbf{x}_i . [It is not enough just to state the formula!] What condition on the Hessian matrix $\nabla^2 f(\mathbf{x}_i) \equiv \mathbf{H}(\mathbf{x}_i)$ needs to hold in order for this strategy to make sense?
- (b) Suppose $\mathbf{x}^* \in \mathbb{R}^n$ satisfies $\nabla f(\mathbf{x}^*) \equiv \mathbf{g}(\mathbf{x}^*) = 0$ with $\mathbf{H}(\mathbf{x}^*)$ positive definite, and \mathbf{H} also satisfies the Lipschitz condition

$$\|\mathbf{H}(\mathbf{x}) - \mathbf{H}(\mathbf{y})\| \leq \gamma(d) \|\mathbf{x} - \mathbf{y}\| \quad \forall \mathbf{x}, \mathbf{y} \in \overline{B}(\mathbf{x}^*, d)$$

for all $d > 0$, where $\overline{B}(\mathbf{x}^*, d) \equiv \{\mathbf{x} \in \mathbb{R}^n : \|\mathbf{x} - \mathbf{x}^*\| \leq d\}$. Carry out the following steps to deduce that the Newton iterates converge quadratically to \mathbf{x}^* from any starting value \mathbf{x}_0 close enough to satisfy

$$\|\mathbf{H}(\mathbf{x}^*)^{-1}\| d_0 \gamma(d_0) < \frac{2}{3},$$

where $d_0 \equiv \|\mathbf{x}_0 - \mathbf{x}^*\|$.

- (i) Assuming the result that, if \mathbf{A}, \mathbf{B} are symmetric $n \times n$ matrices with \mathbf{A} non-singular, then

$$\|\mathbf{A} - \mathbf{B}\| < \frac{1}{\|\mathbf{A}^{-1}\|}$$

implies that \mathbf{B} is also non-singular with

$$\|\mathbf{B}^{-1}\| \leq \frac{\|\mathbf{A}^{-1}\|}{1 - \|\mathbf{A}^{-1}\| \|\mathbf{A} - \mathbf{B}\|};$$

prove that $\mathbf{H}(\mathbf{x})$ is non-singular, and hence positive definite, for $\mathbf{x} \in \overline{B}(\mathbf{x}^*, d_0)$ with

$$\|\mathbf{H}(\mathbf{x})^{-1}\| < 3 \|\mathbf{H}(\mathbf{x}^*)^{-1}\|.$$

- (ii) Use the Newton formula for \mathbf{x}_{i+1} and the integral mean value theorem to prove that, if $\mathbf{x}_i \in \overline{B}(\mathbf{x}^*, d_0)$, then

$$(\dagger) \quad \|\mathbf{x}_{i+1} - \mathbf{x}^*\| < \frac{3}{2} \|\mathbf{H}(\mathbf{x}^*)^{-1}\| \gamma(d_0) \|\mathbf{x}_i - \mathbf{x}^*\|^2.$$

- (iii) Use (\dagger) to prove by induction that the Newton iterates remain in $\overline{B}(\mathbf{x}^*, d_0)$.
- (iv) Use (\dagger) to prove that the Newton iterates converge to \mathbf{x}^* , and hence converge quadratically.

2. (a) Explain carefully one step of the Newton + trust region algorithm for the unconstrained optimisation problem

$$\min f(\mathbf{x}),$$

where $f : \mathbb{R}^n \mapsto \mathbb{R}$ is a smooth function, which may be applied even when the current Hessian matrix fails to be positive definite. Your explanation should include the following points.

- (i) What are the algorithm parameters?
 - (ii) What is the input data at the beginning of the step, and what is the output data ready for the next step?
 - (iii) What is the constrained quadratic optimisation problem that provides a tentative increment? [You do not have to describe how to solve constrained quadratic optimisation problems.]
 - (iv) How does the algorithm decide whether to accept or reject the tentative increment, and what strategy is followed in each case?
- (b) Consider the constrained quadratic optimisation problem

$$\min q(\mathbf{x}) \equiv c - \mathbf{b}^T \mathbf{x} + \frac{1}{2} \mathbf{x}^T \mathbf{G} \mathbf{x} \quad \text{subject to } \|\mathbf{x}\| \leq \Delta,$$

where $q : \mathbb{R}^n \mapsto \mathbb{R}$ with $c \in \mathbb{R}$, $\mathbf{b} \in \mathbb{R}^n$, \mathbf{G} an $n \times n$ symmetric matrix, and $\Delta > 0$. Prove that \mathbf{x}^* solves this problem if and only if $\exists \mu^* \geq 0$ such that

- $[\mathbf{G} + \mu^* \mathbf{I}] \mathbf{x}^* = \mathbf{b}$,
- the complementarity condition $\mu^* [\|\mathbf{x}^*\| - \Delta] = 0$ holds,
- $\mathbf{G} + \mu^* \mathbf{I}$ is positive semi-definite.

In addition, if $\mathbf{G} + \mu^* \mathbf{I}$ is positive definite, show that \mathbf{x}^* is the unique solution of the constrained quadratic optimisation problem.

[You are reminded of the following result, which you may use without proof.

If $f : \mathbb{R}^n \mapsto \mathbb{R}$ and $c : \mathbb{R}^n \mapsto \mathbb{R}$ are smooth functions and $\mathbf{y}^* \in \mathbb{R}^n$ is a local minimum for the inequality constrained problem

$$\begin{aligned} &\min f(\mathbf{x}) \\ &\text{subject to } c(\mathbf{x}) \geq 0, \end{aligned}$$

then $\exists \lambda^* \geq 0$ such that

$$\begin{aligned} \mathbf{g}(\mathbf{y}^*) &= \lambda^* \mathbf{g}_c(\mathbf{y}^*), \quad \lambda^* c(\mathbf{y}^*) = 0 \\ \mathbf{g}_c(\mathbf{y}^*)^T \mathbf{x} &= 0 \quad \Rightarrow \quad \mathbf{x}^T [\mathbf{H}(\mathbf{y}^*) - \lambda^* \mathbf{H}_c(\mathbf{y}^*)] \mathbf{x} \geq 0, \end{aligned}$$

where $\mathbf{g}(\mathbf{x}) \equiv \nabla f(\mathbf{x})$, $\mathbf{H}(\mathbf{x}) \equiv \nabla^2 f(\mathbf{x})$, $\mathbf{g}_c(\mathbf{x}) \equiv \nabla c(\mathbf{x})$ and $\mathbf{H}_c(\mathbf{x}) \equiv \nabla^2 c(\mathbf{x})$.]

3. Consider the linear equality constrained problem

$$(\dagger) \quad \begin{aligned} & \min f(\mathbf{x}) \\ & \text{subject to } \mathbf{Ax} = \mathbf{d}; \end{aligned}$$

where $f : \mathbb{R}^n \mapsto \mathbb{R}$ is a smooth function, $\mathbf{d} \in \mathbb{R}^m$, and $\mathbf{A} \in \mathbb{R}^{m \times n}$ has full rank with $0 < m < n$.

- (a) If the constraint set is denoted

$$\mathcal{S} \equiv \{\mathbf{x} \in \mathbb{R}^n : \mathbf{Ax} = \mathbf{d}\},$$

prove that an equivalent formulation is

$$\mathcal{S} \equiv \{\widehat{\mathbf{x}} + \mathbf{Zv} : \forall \mathbf{v} \in \mathbb{R}^{n-m}\},$$

where $\widehat{\mathbf{x}} \in \mathbb{R}^n$ is a feasible point for (\dagger) and the columns of $\mathbf{Z} \in \mathbb{R}^{n \times (n-m)}$ span the null-space of \mathbf{A} .

- (b) Use this equivalent formulation to explain how (\dagger) may be replaced by an equivalent smaller unconstrained problem

$$(\ddagger) \quad \min \widehat{f}(\mathbf{v}),$$

where $\widehat{f} : \mathbb{R}^{n-m} \mapsto \mathbb{R}$.

- (i) Determine the gradient vectors and Hessian matrices for \widehat{f} in terms of \mathbf{Z} and the gradient vectors and Hessian matrices respectively of f .
- (ii) Hence state the second derivative necessary and sufficient conditions for $\mathbf{x}^* \in \mathcal{S}$ to be a local minimum for (\dagger) .
- (iii) If $\mathbf{x}_i \in \mathcal{S}$, write down the formula for \mathbf{x}_{i+1} when applying Newton's method to (\ddagger) . What condition on the Hessian matrix at \mathbf{x}_i must hold, in order for this formula to make sense?

- (c) For the particular problem with $n = 3$ and $m = 2$,

$$\min f(\mathbf{x}) \equiv x_1^2 + \frac{2}{3}x_2^3 + \frac{2}{3}x_3^3$$

subject to

$$\begin{aligned} x_1 - x_2 + x_3 &= 6 \\ x_1 - 3x_2 - x_3 &= 2 \end{aligned}$$

check that $\mathbf{x}_0 = (4, 0, 2)^T$ is a feasible solution. Use the orthogonal factorisation method to calculate \mathbf{Z} , and hence the projected gradient vector and projected Hessian matrix at \mathbf{x}_0 . Verify that this projected Hessian matrix is positive definite and carry out one step of Newton's method to obtain \mathbf{x}_1 .

[You may use the fact that the orthogonal factorisation is $\mathbf{A} = \mathbf{LQ}$, where

$$\mathbf{L} \equiv \begin{pmatrix} \sqrt{3} & 0 & 0 \\ \sqrt{3} & 2\sqrt{2} & 0 \end{pmatrix} \quad \text{and} \quad \mathbf{Q} \equiv \begin{pmatrix} 1/\sqrt{3} & -1/\sqrt{3} & 1/\sqrt{3} \\ 0 & -1/\sqrt{2} & -1/\sqrt{2} \\ -2/\sqrt{6} & -1/\sqrt{6} & 1/\sqrt{6} \end{pmatrix}.$$

4. Consider the nonlinear inequality constrained problem

$$(\dagger) \quad \begin{aligned} & \min f(\mathbf{x}) \\ & \text{subject to } \mathbf{c}(\mathbf{x}) \geq 0; \end{aligned}$$

where $f : \mathbb{R}^n \mapsto \mathbb{R}$ and $\mathbf{c} : \mathbb{R}^n \mapsto \mathbb{R}^m$ are smooth functions.

- (a) State carefully the KKT conditions, which are necessary for $\mathbf{x}^* \in \mathbb{R}^n$ to be a local minimum of (\dagger) ; using $\mathbf{g}(\mathbf{x}^*) \equiv \nabla f(\mathbf{x}^*) \in \mathbb{R}^n$ to denote the gradient vector of f at \mathbf{x}^* and $\mathbf{g}_i(\mathbf{x}^*) \equiv \nabla c_i(\mathbf{x}^*) \in \mathbb{R}^n$ to denote the gradient vector of the i^{th} component of \mathbf{c} at \mathbf{x}^* .
- (b) Consider the following particular example of (\dagger) with $n = 2$ and $m = 4$:

$$(\ddagger) \quad f(\mathbf{x}) \equiv (x_1 - \frac{3}{2})^2 + (x_2 - \frac{1}{2})^4 \quad \text{and} \quad \mathbf{c}(\mathbf{x}) \equiv \begin{pmatrix} 1 - x_1 - x_2 \\ 1 - x_1 + x_2 \\ 1 + x_1 - x_2 \\ 1 + x_1 + x_2 \end{pmatrix}.$$

- (i) Draw the feasible set in \mathbb{R}^2 for these inequality constraints.
- (ii) Write down the KKT conditions for (\ddagger) .
- (iii) By carefully considering all the allowed possibilities for zero Lagrange multipliers, determine the unique solution $\mathbf{x}^* \in \mathbb{R}^2$ for these KKT equations. Make sure you state which constraints are active at \mathbf{x}^* and give the values for the corresponding Lagrange multipliers.