Scientific Computing (COMP3407)
Programming Assignment 2

Start: Mar. 8, 2019 Due: 22:00, Mar. 22, 2019

1 Linear Least Squares and QR Decomposition (50 marks)

(a) (5 marks) Please write a function to compute the Householder reflection Q_u that maps a vector $\mathbf{x}$ to another vector $\mathbf{y}$ of the same length in R^n. The function should take two vectors $\mathbf{x}$ and $\mathbf{y}$ as input and produce the corresponding orthogonal matrix Q_u as output. Your program should print an error message if the input vectors are zero vectors or have different lengths. When $\mathbf{x} = \mathbf{y}$, an identity matrix should be returned.

(b) (25 marks) Please write a function to compute the QR decomposition of a matrix A using the Householder reflection. Given a full-rank matrix $\mathrm{A} \in \mathbb{R}^{m\times n}$ $(m \geq n)$, your program should be able to decompose it to the form

$$\mathrm{A} = \mathrm{Q}\begin{pmatrix} \mathrm{R} \\ 0 \end{pmatrix}$$

where $\mathrm{Q} \in \mathbb{R}^{m\times m}$ is orthogonal and $\mathrm{R} \in \mathbb{R}^{n\times n}$ is an upper triangular matrix. Your program should take an arbitrarily matrix A as input. The orthogonal matrix Q and the upper triangular matrix **R** should be returned if no zero column vector is encountered during the decompostion process; otherwise, the program should print an error message to indicate that A is not full-rank.

(c) (10 marks) Use QR decomposition to solve the following linear system

$$\begin{pmatrix} 6 & 1 & & & & & \\ 8 & 6 & 1 & & & & \\ & 8 & 6 & 1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & 8 & 6 & 1 & \\ & & & & 8 & 6 & 1 \\ & & & & & 8 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{82} \\ x_{83} \\ x_{84} \end{pmatrix} = \begin{pmatrix} 7 \\ 15 \\ 15 \\ \vdots \\ 15 \\ 15 \\ 14 \end{pmatrix}$$

Print the solution $\hat{\mathbf{x}}$ and the 2-norm of the residual $\mathbf{r} = \mathrm{A}\hat{\mathbf{x}} - \mathbf{b}$.

(d) (10 marks) Use QR decomposition to solve the following least squares problem. Given the data below, compute a quadratic polynomial $f = at^2 + bt + c$ to minimize the 2-norm of the residual vector $\mathbf{r} = \mathbf{y} - f(\mathbf{t})$.

t_i	-1	-0.75	-0.5	0	0.25	0.5	0.75
y_i	1.0000	0.8125	0.7500	1.0000	1.3125	1.7500	2.3125

2 Fixed-point Iteration (20 marks)

Using the fixed-point iteration to compute the value of the following expressions. Discuss your choice of the initial values and the convergence of the iterations.
(a) (10 marks)

$$x = \sqrt{2 + \sqrt{2 + \sqrt{2 + \cdots}}}$$

(b) (10 marks)

$$x = \cfrac{1}{1 + \cfrac{1}{1 + \cfrac{1}{1 + \cdots}}}$$

3 Non-linear equations (30 marks)

Implement the bisection method and Newton's method for solving univariate nonlinear equations, and test your implementations by finding a root of each of the following equations.

(a) $x^3 - 2x - 5 = 0$ on $[2, 4]$ or near 4

(b) $e^{-x} = x$ on $[0, 2]$ or near 2

(c) $x\sin(x) = 1$ on $[0, 2]$ or near 0

(d) $x = \tan(x)$ on $[4, 6]$ or near 4

Please use the suggested initial intervals for the bisection method and the suggested initial values for Newton's method. Generate a plot for each equation which gives the errors of the two methods with respect to the number of iterations. You may use the MATLAB command **legend** to distinguish the plots of two methods.

4 (Bonus Question) A Variation of Backward Substitution (20 marks)

Suppose that $\lambda \in \mathbb{R}$ is a constant, $\mathrm{S}, \mathrm{T} \in \mathbb{R}^{n\times n}$ are two upper triangular matrices and $\mathrm{ST} - \lambda\mathrm{I}$ is nonsingular. Note that S and T are not necessarily nonsingular. It is clear that the straightforward matrix multiplication has $\mathcal{O}(n^3)$ time complexity. Please give an algorithm with $\mathcal{O}(n^2)$ time complexity to solve the linear system $(\mathrm{ST} - \lambda\mathrm{I})\mathbf{x} = \mathbf{b}$ without computing the multiplication of S and T. Write a function in MATLAB to implement your method. (Hint: There are two ways to solve it: (1) divide and conquer; (2) interchange the order of summation.)