18.085 Computational Science and Engineering
Problem Set 2
Due in-class on 5th March 2015

Clarification required? Email `ajt@mit.edu`

1. (10 marks) Here is an example of a "reduced" QR factorization of a rectangular matrix:

$$\begin{pmatrix} 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{pmatrix} = \begin{pmatrix} \sqrt{3}/3 & -\sqrt{2}/2 \\ \sqrt{3}/3 & 0 \\ \sqrt{3}/3 & \sqrt{2}/2 \end{pmatrix} \begin{pmatrix} \sqrt{3} & 3\sqrt{3} \\ 0 & \sqrt{2} \end{pmatrix}.$$

   Verify in this example that $A^TA = R^TR$. (Therefore, the normal equations $A^TAx = A^Tb$ become $Rx = Q^Tb$.) By solving the normal equations, find the best-fit line $y = c + dx$ to the data $(x, y) = (2, 3), (3, 3), (4, 6)$.

2. (10 marks) Here are two matrices:

$$A = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \qquad B = \begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 0 & 1 \end{pmatrix}.$$

   Showing your hand calculations, find a $PA = LU$ decomposition of A and find the upper-triangular matrix R in a $B = QR$ decomposition of B (Q is square). (Hint: If Q is orthogonal then $\|Qx\|_2 = \|x\|_2$ for any vector x.)

3. (10 marks) The 2nd order differential equation $-u''(x) = f(x)$, $u'(0) = 0$, $u(1) = 0$ has the following $n \times n$ matrix discretization:

$$\underbrace{\begin{pmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & \ddots & \ddots & \\ & & \ddots & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}}_{T_n} \underbrace{\begin{pmatrix} u(0) \\ u(h) \\ \vdots \\ u((n-2)h) \\ u((n-1)h) \end{pmatrix}}_{v} = \underbrace{\begin{pmatrix} h^2 f(0) \\ h^2 f(h) \\ \vdots \\ h^2 f((n-2)h) \\ h^2 f((n-1)h) \end{pmatrix}}_{b},$$

where $h = 1/(n+1)$. Write down the LU decomposition of T_n (do T_3, T_4, T_5, ... to get the pattern if you wish). Use the LU decomposition to solve $T_3 v = (1,1,1)^T/16$. Describe in general how you would solve $T_n v = b$ using $T_n = LU$.
(Bonus part, hard but interesting, extra 2 marks) By recalling the forward and backward difference formulas,

$$u'(x) \approx \frac{u(x+h) - u(x)}{h}, \qquad u'(x) \approx \frac{u(x) - u(x-h)}{h},$$

what is the corresponding process when directly solving the differential equation (without discretizing)?

4. (10 marks) Let A be an $n \times n$ square matrix and suppose $A = Q_1 R_1 = Q_2 R_2$, where Q_1 and Q_2 are orthogonal matrices and R_1 and R_2 are upper-triangular matrices.
(a) Show that $Q_2^T Q_1$ is an orthogonal matrix.
(b) Show that $Q_2^T Q_1 = R_2 R_1^{-1}$.
(c) If D is an upper-triangular orthogonal matrix, show that D must be a diagonal matrix where each diagonal entry is $+1$ or -1.
(d) By setting $B = Q_2^T Q_1 = R_2 R_1^{-1}$, what form does B take? (Note that $R_2 R_1^{-1}$ is an upper-triangular matrix.)
(e) [Challenging] How many QR factorizations does A have?

5. (Totally for fun, no extra marks, only brownie points) Download the dataset `LoadBMIData.m` from the course website. By using least squares, or otherwise, derive your own model for how weight and height are related for Hong Kong children.