Math 5660 Fall 2001 Jan Mandel

Least squares and QR

Problem:
Given $A \in \Re^{m\times n}$ and $b \in R^m$, $m \geq n$, find x such that $\|Ax - b\|$ is mininal. This x is called the *least squares* solution of $Ax = b$.

Solution:
Let $x, h \in \Re^n$, and let $f(t) = \|A(x+th)-b\|^2 = (A(x+th)-b)^T(A(x+th)-b)$. By a direct computation (done in class), $f'(0) = h^T(A^TAx - A^Tb)$. The number $f'(0)$ is the derivative of $\|Ax-b\|^2$ in the direction h. It is known that if $\|Ax-b\|^2$ is minimal then all directional derivatives are zero, hence $h^T(A^TAx - A^Tb) = 0$ for all h. This implies that the solution x of the minimization problem satisfies the system of equations

$$A^TAx = A^Tb,$$

called the *normal equations.*
The QR decomposition of A gives $A = QR$, where $Q \in \Re^{m\times m}$ is unitary and $R \in \Re^{m\times n}$ is upper triangular, that is

$$R = \begin{bmatrix} L^T \\ 0 \end{bmatrix},$$

where $L^T \in \Re^{n\times n}$ (that is, L^T is the same size as A^TA). Then

$$A^TA = R^TQ^TQR = R^TR = LL^T,$$

that is, L is the Choleski factor of A^TA. If the columns of A are linearly independent, then A^TA is nonsingular, and the normal equations can be solved by solving in turn the two nonsingular triangular systems $Ly = A^Tb, \quad L^Tx = y$.

Homework:
Let

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

.

1. Compute by hand the QR decomposition of A. Use the algorithm from the book. Compute both Q and R.
2. Find the least squares solution of $Ax = b$.
3. Verify the results in Matlab, that is, compute $A - QR$, $Q^TQ - I$, and $A^TAx - A^Tb$ for your hand calculated results. You may but do not need to print the Matlab log, you can just copy the results by hand.