Linear Least Squares Computations

Assuming that $A \in \mathbb{R}^{m \times n}$ has linearly independent columns, the problem

$$\arg\min_x \|Ax - b\|_2 \tag{1}$$

has a unique solution, say x_{LS}, which is also the unique solution to the normal equations

$$A^T Ax = A^T b. \tag{2}$$

This suggests the *normal equations approach* to computing x_{LS}:

1. Form $C = A^T A$, and $w = A^T b$.
2. Compute the Cholesky factorization $C = LL^T$.
3. Solve $Ly = w$ by forsub and then $L^T x = y$ by backsub.

This algorithm requires $mn^2 + \frac{1}{3}n^3 + O(mn)$ flops (taking advantage of the symmetry of C). It is an important method because it is fast and doesn't use very much memory. $Cx = w$ can be viewed as a compressed form of $\arg\min_x \|Ax - b\|_2$.

We have other methods that, while more costly, are more robust in the face of rounding errors. The other methods arrive at x_{LS} by a different route. Recall that the normal equations were a result of requiring that $b - Ax$ be orthogonal (normal) to the subspace $S = \mathrm{ColSp}(A)$. That is another way of saying that Ax is the orthogonal projection of b onto S. The solution to the normal equations is therefore the solution to the rectangular, but consistent, linear system

$$Ax = Pb, \tag{3}$$

where P is the orthogonal projector onto $S = \mathrm{ColSp}(A)$.

Now if Z is *any* matrix whose columns form a basis for S, then the orthogonal projector onto S is $P = Z(Z^T Z)^{-1} Z^T$, and (3) becomes

$$Ax = Z(Z^T Z)^{-1} Z^T b. \tag{4}$$

This family of equations, parametrized by Z, explains most methods. For example, the normal equations gives $x = (A^T A)^{-1} A^T b$, and premultiplying by A gives $Ax = A(A^T A)^{-1} A^T b$, which is (4), with $Z = A$.

The most often used LS methods compute a matrix $Z = Q$ whose columns form an orthonormal basis for S. Since Q and A have the same column space, each column of A is a linear combination of the columns of Q. That is $A = QR$, where $R \in \mathbb{R}^{n \times n}$, and (3) becomes $QRx = QQ^T b$. Premultiplying by Q^T gives the (smaller and nonsingular) $n \times n$ system

$$Rx = Q^T b.$$