Theorem 6.3 *Let A be an $n \times k$ matrix and let $r = rank(A)$. Then there exist a matrix Q of dimensions $n \times r$ consisting of orthonormal columns and an upper triangular matrix R of dimension $r \times k$ such that the following properties hold*

- $A = QR$
- $R(A) = R(Q)$. *In particular, the columns of Q form an orthonormal basis in $R(A)$, hence $Q^tQ = I$. The matrix $P = QQ^t$ is the orthogonal projection from $\mathbf{R}^n$ onto $R(A)$.*
- $Ker\,A = Ker\,R$, *in particular $rank(R) = r$.*

Finally, it is always possible to ensure that the first nonzero elements in each row of R be nonnegative. With this extra requirement, such a decomposition is unique.

While the LU and QR factors can be used in more or less the same way to solve nonsingular systems, things are different for singular and rectangular cases because $\mathbf{Ax} = \mathbf{b}$ might be inconsistent, in which case a least squares solution as described in §4.6, (p. 223) may be desired. Unfortunately, the LU factors of $\mathbf{A}$ don't exist when $\mathbf{A}$ is rectangular. And even if $\mathbf{A}$ is square and has an LU factorization, the LU factors of $\mathbf{A}$ are not much help in solving the system of normal equations $\mathbf{A}^T\mathbf{Ax} = \mathbf{A}^T\mathbf{b}$ that produces least squares solutions. But

the QR factors of $\mathbf{A}_{m\times n}$ always exist as long as $\mathbf{A}$ has linearly independent columns, and, as demonstrated in the following example, the QR factors provide the least squares solution of an inconsistent system in exactly the same way as they provide the solution of a consistent system.

Application to the Least Squares Problem. If $\mathbf{Ax} = \mathbf{b}$ is a possibly inconsistent (real) system, then, as discussed on p. 226, the set of all least squares solutions is the set of solutions to the system of normal equations

$$\mathbf{A}^T\mathbf{Ax} = \mathbf{A}^T\mathbf{b}. \tag{5.5.5}$$

But computing $\mathbf{A}^T\mathbf{A}$ and then performing an LU factorization of $\mathbf{A}^T\mathbf{A}$ to solve (5.5.5) is generally not advisable. First, it's inefficient and, second, as pointed out in Example 4.5.1, computing $\mathbf{A}^T\mathbf{A}$ with floating-point arithmetic can result in a loss of significant information. The QR approach doesn't suffer from either of these objections. Suppose that $rank\,(\mathbf{A}_{m\times n}) = n$ (so that there is a unique least squares solution), and let $\mathbf{A} = \mathbf{QR}$ be the QR factorization. Because the columns of $\mathbf{Q}$ are an orthonormal set, it follows that $\mathbf{Q}^T\mathbf{Q} = \mathbf{I}_n$, so

$$\mathbf{A}^T\mathbf{A} = (\mathbf{QR})^T(\mathbf{QR}) = \mathbf{R}^T\mathbf{Q}^T\mathbf{QR} = \mathbf{R}^T\mathbf{R}. \tag{5.5.6}$$

Consequently, the normal equations (5.5.5) can be written as

$$\mathbf{R}^T\mathbf{Rx} = \mathbf{R}^T\mathbf{Q}^T\mathbf{b}. \tag{5.5.7}$$

But $\mathbf{R}^T$ is nonsingular (it is triangular with positive diagonal entries), so (5.5.7) simplifies to become

$$\mathbf{Rx} = \mathbf{Q}^T\mathbf{b}. \tag{5.5.8}$$

This is just an upper-triangular system that is efficiently solved by back substitution. In other words, most of the work involved in solving the least squares problem is in computing the QR factorization of $\mathbf{A}$. Finally, notice that

$$\mathbf{x} = \mathbf{R}^{-1}\mathbf{Q}^T\mathbf{b} = \left(\mathbf{A}^T\mathbf{A}\right)^{-1}\mathbf{A}^T\mathbf{b}$$

is the solution of $\mathbf{Ax} = \mathbf{b}$ when the system is consistent as well as the least squares solution when the system is inconsistent (see p. 214). That is, with the QR approach, it makes no difference whether or not $\mathbf{Ax} = \mathbf{b}$ is consistent because in both cases things boil down to solving the same equation—namely, (5.5.8). Below is a formal summary.

Linear Systems and the QR Factorization

If $rank\,(\mathbf{A}_{m\times n}) = n$, and if $\mathbf{A} = \mathbf{QR}$ is the QR factorization, then the solution of the nonsingular triangular system

$$\mathbf{Rx} = \mathbf{Q}^T\mathbf{b} \tag{5.5.9}$$

is either the solution or the least squares solution of $\mathbf{Ax} = \mathbf{b}$ depending on whether or not $\mathbf{Ax} = \mathbf{b}$ is consistent.

It's worthwhile to reemphasize that the QR approach to the least squares problem obviates the need to explicitly compute the product $\mathbf{A}^T\mathbf{A}$. But if $\mathbf{A}^T\mathbf{A}$ is ever needed, it is retrievable from the factorization $\mathbf{A}^T\mathbf{A} = \mathbf{R}^T\mathbf{R}$. In fact, this is the ***Cholesky factorization*** of $\mathbf{A}^T\mathbf{A}$ as discussed in Example 3.10.7, p. 154.

Now let's consider some examples: Let's first consider fitting a line to three points. supoose the three points are

$$(1,2) \quad (2,5) \quad (3,7)\ .$$

$$A = \begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 3 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{b} = \begin{bmatrix} 2 \\ 5 \\ 7 \end{bmatrix}\ .$$

Let $\mathbf{v}_1$ and $\mathbf{v}_2$ be the first and second columns of A. Doing Gram–Schmidt, we normalize the first column of A getting

$$\mathbf{u}_1 = \frac{1}{|\mathbf{v}_1|}\mathbf{v}_1 = \frac{1}{\sqrt{14}}\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}\ . \tag{11}$$

Then we form

$$\mathbf{w}_2 = \mathbf{v}_2 - (\mathbf{u}_1\cdot\mathbf{v}_2)\mathbf{u}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} - \frac{6}{\sqrt{14}}\frac{1}{\sqrt{14}}\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} = \frac{1}{7}\begin{bmatrix} 4 \\ 1 \\ -2 \end{bmatrix}\ . \tag{12}$$

Now normalize this to get

$$\mathbf{u}_2 = \frac{1}{|\mathbf{w}_2|}\mathbf{w}_2 = \frac{1}{\sqrt{21}} \begin{bmatrix} 4 \\ 1 \\ -2 \end{bmatrix} \ . \tag{13}$$

This gives us

$$Q = \frac{1}{\sqrt{42}} \begin{bmatrix} \sqrt{3} & 4\sqrt{2} \\ 2\sqrt{3} & \sqrt{2} \\ 3\sqrt{3} & -2\sqrt{2} \end{bmatrix} \ .$$

Finally, (10) tells us that

$$\mathbf{v}_1 = \sqrt{14}\mathbf{u}_1$$

so the first column of R is

$$\begin{bmatrix} \sqrt{14} \\ 0 \end{bmatrix} \ .$$

Next, from (12) and (13), we have

$$\mathbf{v}_2 = (\mathbf{u}_1 \cdot \mathbf{v}_2)\mathbf{u}_1 + |\mathbf{w}_2|\mathbf{u}_2 = \frac{6}{\sqrt{14}}\mathbf{u}_1 + \frac{\sqrt{21}}{7}\mathbf{u}_2$$

and so the second column of R is

$$\begin{bmatrix} \frac{6}{\sqrt{14}} \\ \frac{\sqrt{21}}{7} \end{bmatrix} \ .$$

Thus

$$R = \begin{bmatrix} \sqrt{14} & \frac{6}{\sqrt{14}} \\ 0 & \frac{\sqrt{21}}{7} \end{bmatrix} \ .$$

Alternatively, for any M by n matrix, $A = QR$ just means that

$$\mathbf{v}_j = \sum_{\ell=1}^{m} \mathbf{u}_\ell R_{\ell j}$$

by the "column picture" for matrix multiplication. Taking the dot product with $\mathbf{u}_i$ and using the definition of orthogonality,

$$\mathbf{u}_i \cdot \mathbf{v}_j = \mathbf{u}_i \cdot \left(\sum_{\ell=1}^{m} \mathbf{u}_\ell R_{\ell j} \right) = \sum_{\ell=1}^{m} R_{\ell j} \mathbf{u}_i \cdot \mathbf{u}_\ell = R_{ij} \ .$$

So once you have all of the $\mathbf{u}_i$ computed, you can compute the entries of R using

$$R_{ij} = \mathbf{u}_i \cdot \mathbf{v}_j \ . \tag{14}$$

Either way, the point is that once you've got the $\mathbf{u}_i$ computed, you've also got both Q and R at your fingertips.

Next, compute

$$Q^t \mathbf{b} = \begin{bmatrix} \frac{33}{\sqrt{14}} \\ \frac{-1}{\sqrt{21}} \end{bmatrix} \ ,$$

and then solve

$$R\mathbf{x} = \begin{bmatrix} \frac{33}{\sqrt{14}} \\ \frac{-1}{\sqrt{21}} \end{bmatrix} \ .$$

The answer is

$$\mathbf{x} = \begin{bmatrix} \frac{5}{2} \\ \frac{-1}{3} \end{bmatrix} \ .$$

The best fit line is therefore

$$y = \frac{5}{2}x - \frac{1}{3} \ .$$

Here is a picture of the best fit line plotted together with the data points:

Next, consider a more realistic example, in which the data points are not all integer. Suppose our data points (x_i, y_i), $i = 1, 2, \ldots, 5$ are

$$(1, 1.9) \quad (2, 3.7) \quad (3, 6.2) \quad (4, 7.7) \quad (5, 10.5) \ .$$

Then

$$A = \begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 3 & 1 \\ 4 & 1 \\ 5 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{b} = \begin{bmatrix} 1.9 \\ 3.7 \\ 6.2 \\ 7.7 \\ 10.5 \end{bmatrix}$$

Doing the Gram-Schmidt procedure yields $A = QR$ where

$$Q = \frac{1}{\sqrt{55}} \begin{bmatrix} 1 & 4\sqrt{2} \\ 2 & \frac{5}{\sqrt{2}} \\ 3 & \sqrt{2} \\ 4 & \frac{-1}{\sqrt{2}} \\ 5 & \frac{-2}{\sqrt{2}} \end{bmatrix}$$

and

$$R = \begin{bmatrix} 1 & \frac{3}{11} \\ 0 & \frac{\sqrt{2}}{11} \end{bmatrix} \ .$$

Next compute

$$Q^t\mathbf{b} = \frac{\sqrt{55}}{275} \begin{bmatrix} 556 \\ -9\sqrt{2} \end{bmatrix} \ .$$

Finally, solving $R\mathbf{x} = Q^t\mathbf{b}$ simply means solving the 2 by 2 upper triangular system

$$\begin{bmatrix} 1 & \frac{3}{11} \\ 0 & \frac{\sqrt{2}}{11} \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \frac{\sqrt{55}}{275} \begin{bmatrix} 556 \\ -9\sqrt{2} \end{bmatrix} \ .$$

Since R is upper triangular, we can read off the value of b right away, and solving for a we get

$$a = \frac{53}{25} \qquad \text{and} \qquad b = \frac{-9}{25} \ .$$

Now let's consider another example. Let's find a good polynomial fit to $\sin(x)$ on $0 \le x \le \pi/2$. Since this is an odd function, we will use a linear combination of odd powers of x. If we use the first four odd powers, this means finding values of a, b, c and d so that

$$\sin(x) \approx ax + bx^3 + cx^5 + dx^7 \quad \text{for} \quad 0 \le x \le \frac{\pi}{2}$$

Now we know

$$\sin(\pi/6) = \frac{1}{2} \qquad \sin(\pi/4) = \frac{1}{\sqrt{2}} \qquad \sin(\pi/3) = \frac{\sqrt{3}}{2} \qquad \sin(\pi/2) = 1 \ .$$

From the angle addition formula we have

$$\sin(5\pi/12) = \sin(\pi/3 + \pi/4) = \frac{\sqrt{3}+1}{2\sqrt{2}}$$

and

$$\sin(\pi/12) = \sin(\pi/3 - \pi/4) = \frac{\sqrt{3}-1}{2\sqrt{2}} \ .$$

Therfore we define

$$x_1 = \frac{\pi}{12} \quad x_2 = \frac{\pi}{6} \quad x_3 = \frac{\pi}{4} \quad x_4 = \frac{\pi}{3} \quad x_5 = \frac{5\pi}{12} \quad x_6 = \frac{\pi}{2}$$

and

$$y_1 = \sin\frac{\pi}{12} \quad y_2 = \sin\frac{\pi}{6} \quad y_3 = \sin\frac{\pi}{4} \quad y_4 = \sin\frac{\pi}{3} \quad y_5 = \sin\frac{5\pi}{12} \quad y_6 = \sin\frac{\pi}{2}$$

The matrix A is now

$$A = \begin{bmatrix} x_1 & x_1^3 & x_1^5 & x_1^7 \\ x_2 & x_2^3 & x_2^5 & x_2^7 \\ x_3 & x_3^3 & x_3^5 & x_3^7 \\ x_4 & x_4^3 & x_4^5 & x_4^7 \\ x_5 & x_5^3 & x_5^5 & x_5^7 \\ x_6 & x_6^3 & x_6^5 & x_6^7 \end{bmatrix}$$

yielding

$$f(x) = (.9999976966)x - (.1666522644)x^3 + (.008309725100)x^5 - (.0001844086724)x^7 \ .$$

If we plot this from 0 to $\pi/2$, the graph is inditinguishable to the eye from that of $\sin(x)$, but if we plot from 0 to π, we can see the two graphs pull apart.