Least squares problems and QR factorization

Alternative way to solve linear least-squares problems: start from

ortho tri

$$\underbrace{A = QR}, \quad Q = {}^{m}\begin{array}{cc} n & m-n \\ \left[\, Q_1 \right. & \left. \vdots \; Q_2 \,\right] \end{array}, \quad R = \begin{bmatrix} R_1 \\ 0 \end{bmatrix} \begin{array}{l} n \\ m-n \end{array}.$$

$A = QR = Q_1 \cdot R_1 + Q_2 \cdot 0 = Q_1 R_1$

Trick: since orthogonal matrices preserve norm-2,

$$\begin{aligned}
\|Ax - b\| &= \|Q^T(Ax - b)\| = \|Q^T QRx - Q^T b\| \\
&= \|Rx - Q^T b\| = \left\| \begin{bmatrix} R_1 \\ 0 \end{bmatrix} x - \begin{bmatrix} Q_1^T \\ Q_2^T \end{bmatrix} b \right\| \\
&= \left\| \begin{bmatrix} R_1 x - Q_1^T b \\ Q_2^T b \end{bmatrix} \right\|.
\end{aligned}$$

For every vector $\underline{x \in \mathbb{R}^n}$ $\qquad A = Q \cdot R$

$$\|\underbrace{Ax-b}\| = \|Q^T(\underbrace{Ax-b})\| = \|\underbrace{Q^T Q}_{= I} R x - Q^T b\| =$$

$$= \|Rx - Q^T b\| = \left\| \begin{bmatrix} R_1 \\ 0 \end{bmatrix} x - \begin{bmatrix} Q_1^T \\ Q_2^T \end{bmatrix} b \right\| =$$

$$= \left\| \begin{bmatrix} R_1 x \\ 0 \end{bmatrix} - \begin{bmatrix} Q_1^T b \\ Q_2^T b \end{bmatrix} \right\| = \left\| \begin{bmatrix} R_1 x - Q_1^T b \\ -Q_2^T b \end{bmatrix} \right\|$$

depends on x

does not depend on x

$$\left\| \begin{bmatrix} R_1 x - Q_1^T b \\ \hline -Q_2^T b \end{bmatrix} \right\| \geq \|Q_2^T b\|$$

$$\left\| \begin{bmatrix} c(x) \\ d \end{bmatrix} \right\| = \sqrt{c_1^2 + c_2^2 + \dots + c_n^2 + d_1^2 + \dots d_{m-n}^2}$$

$\geq \sqrt{d_1^2 + \dots + d_{m-n}^2}$

If I choose x s.t. $\boxed{R_1 x = Q_1^T b}$

then the first block $R_1 x - Q_1^T b$ becomes 0

$\Rightarrow$ the value of x such that $R_1 x = Q_1^T b$ is the solution of the LS problem

$$\boxed{x = R_1^{-1} Q_1^T b}$$

$\uparrow$

$n \times n$

Solving least squares with QR

$$\|Ax - b\| = \left\| \begin{bmatrix} R_1 x - Q_1^T b \\ Q_2^T b \end{bmatrix} \right\|$$

How can we minimize the norm of this vector?

Bottom block: same value, regardless of x. The squares of those entries will always be in the sum.

Top block I can choose x to make its entries smaller. Can I get $R_1 x - Q_1^T b = 0$? Yes, if R_1 invertible.

When is R_1 invertible?

Related to a result we have seen earlier. If $A = QR$, with Q orthogonal, then

$$A^T A = (QR)^T (QR) = R^T \underbrace{Q^T Q}_{=I} R = R^T R = \begin{bmatrix} R_1^T & 0 \end{bmatrix} \begin{bmatrix} R_1 \\ 0 \end{bmatrix} = R_1^T R_1.$$

A has full column rank $\iff$ $A^T A$ is posdef $\iff$ $A^T A = R_1^T R_1$ is invertible $\iff$ R_1 is inverbile.

(Note for the future: $R_1^T R_1$ is the Cholesky factorization of $A^T A$.)

Is R_1 invertible? $\qquad A = QR = Q_1R_1$

$$\underbrace{A^TA} = (R^TQ^T)(QR) = R^T(\underbrace{Q^TQ}_{I})R = R^TR =$$

$$= [R_1^T \ 0] \cdot \begin{bmatrix} R_1 \\ 0 \end{bmatrix} = R_1^TR_1 + 0 \cdot 0 = \underbrace{R_1^TR_1}$$

A has full col. rank $\Leftrightarrow$ A^TA is pos. def

$\Leftrightarrow$ A^TA is invertible $\Leftrightarrow$ $R_1^TR_1$ is invertible

$\Leftrightarrow$ R_1 is invertible

(*)

A^TA is posdef if it has no 0 eigenvalue

(*) If R_1 invertible, then $(R_1^T R_1)^{-1} = R_1^{-1}(R_1^T)^{-1}$

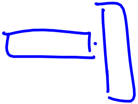
$\Rightarrow R_1^T R_1$ is invertible

If R_1 is singular (not invertible), then $R_1^T R_1$ is not invertible

$$\det(R_1^T R_1) = \det(R_1^T)\det R_1$$

if this is zero...

then this is zero as well



$A^T A$

$\square \cdot \square$

$R_1^T R_1$

Rmk: Steps in red make sense only because R_1 is square

Recap

If $A = QR = \begin{bmatrix} Q_1 & Q_2 \end{bmatrix} \begin{bmatrix} R_1 \\ 0 \end{bmatrix}$ (and has full column rank), then the solution of $\min \|Ax - b\|$ is given by $x = R_1^{-1}(Q_1^T)b$.

Note that 'thin QR' $A = Q_1 R_1$ contains all we need here.

This gives (of course) the same solution x as the normal equations method. Indeed, some algebra gives

$$(A^T A)x = A^T b$$

$$A^T A = R_1^T R_1, \quad A^T b = R_1 Q_1^T b.$$

so the two methods solve similar linear systems:

Normal equations	QR-based method
$R_1^T R_1 x = R_1^T Q_1^T b$	$R_1 x = Q_1^T b.$

Exercises

1. Is it true that every symmetric, positive definite matrix $M \in \mathbb{R}^{m \times m}$ can be written as $B^T B$ for some $B \in \mathbb{R}^{m \times m}$? Hint: start from eigendecomposition $M = Q \Lambda Q^T$, and consider $\begin{bmatrix} \sqrt{\lambda_1} & & \\ & \ddots & \\ & & \sqrt{\lambda_m} \end{bmatrix}$.