Combining QR Decomposition and Normal Equation

QR Decomposition is

$$A = \underbrace{Q}_{\text{orthogonal columns}}\ \underbrace{R}_{\text{square, upper triangular (with 1 on diag)}}$$

Plug this into Normal Eqn:

$$A\underline{x} = \underline{b}$$

best approx. solution

$$A^TA\,\hat{\underline{x}} = A^Tb$$

$$(QR)^T(QR)\,\hat{\underline{x}} = (QR)^T\underline{b}$$

Note: Transpose reverses order of multiplication!

$$A \cdot B = [(\text{row } A)\bullet(\text{col } B)]$$

$$[(\text{row } B^T)\bullet(\text{col } A^T)] = B^TA^T$$

$$R^T\underbrace{Q^TQ}_{\text{diagonal}}R\,\hat{\underline{x}} = R^TQ^T\underline{b}$$

$$R^TDR\,\hat{\underline{x}} = R^TQ^T\underline{b}$$

(continuing...)

$$\cancel{R^T}DR\,\hat{\underline{x}} = \cancel{R^T}Q^T\underline{b}$$

R^T is square, lower Δ with 1 on the diagonal so it is "invertible" — these cancel

$$DR\,\hat{\underline{x}} = \underbrace{Q^T\underline{b}}_{\text{dot product of columns of } Q \text{ with } \underline{b}}$$

$$R\,\hat{\underline{x}} = \underbrace{D^{-1}}_{\text{divide by dot product of columns of } Q \text{ with themself}}Q^Tb$$

$$Q = \begin{bmatrix} | & | & \\ q_1 & q_2 & \cdots \\ | & | & \end{bmatrix}$$

$$\boxed{R\,\hat{\underline{x}} = \begin{bmatrix} \frac{b\cdot q_1}{q_1\cdot q_1} \\ \frac{b\cdot q_2}{q_2\cdot q_2} \\ \vdots \end{bmatrix}}$$

Note: Division by R is easy because R is square, upper triangular with 1 on diagonal.

Example: Find best approximate solution to

$$\begin{bmatrix} -5 & -3 & 0 \\ -2 & -4 & 1 \\ 4 & -1 & 1 \\ 5 & 4 & -1 \end{bmatrix} \underline{\underline{x}} = \begin{bmatrix} -1 \\ -3 \\ -3 \\ 0 \end{bmatrix}$$

using the QR-Decomposition

$$\begin{bmatrix} -5 & -3 & 0 \\ -2 & -4 & 1 \\ 4 & -1 & 1 \\ 5 & 4 & -1 \end{bmatrix} = \begin{array}{c} \begin{bmatrix} 1 & -3 & 0 \\ 1 & -1 & 1 \\ 1 & 2 & 1 \\ 2 & 1 & -1 \end{bmatrix} \\ \begin{matrix} q_1 & q_2 & q_3 \end{matrix} \end{array} \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & -3 & 1 \end{bmatrix}}_{R}$$

The normal eqn becomes $R\hat{\underline{\underline{x}}} = \begin{bmatrix} \frac{b\cdot q_1}{q_1\cdot q_1} \\ \frac{b\cdot q_2}{q_2\cdot q_2} \\ \vdots \end{bmatrix}$

$$\begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & -3 & 1 \end{bmatrix} \hat{\underline{\underline{x}}} = \begin{bmatrix} \frac{-1-3-3}{1+1+1+4} \\ \frac{3+3-6}{9+1+4+1} \\ \frac{-3-3}{1+1+1} \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & -3 & 1 \end{bmatrix} \hat{\underline{\underline{x}}} = \begin{bmatrix} -1 \\ 0 \\ -2 \end{bmatrix}$$

Divide using "Forward Substitution":

$x_1 = -1$

$2x_1 + x_2 = 0 \implies x_2 = 2$

$-x_1 - 3x_2 + x_3 = -2 \implies x_3 = 3$

$$\hat{\underline{\underline{x}}} = \begin{bmatrix} -1 \\ 2 \\ 3 \end{bmatrix}$$

Extra Note: If A is square, then QR decomposition won't just find the best "approximate" solution — it will find *the* solution.

[Unless $A\underline{\underline{x}} = \underline{\underline{b}}$ has more than one solution... in that case, the columns of A will not be independent so Q will have columns of all 0 at the start...]