Least-Squares Systems and The QR factorization

- **Orthogonality**
- **Least-squares systems.**
- **The Gram-Schmidt and Modified Gram-Schmidt processes.**
- **The Householder QR and the Givens QR.**

Orthogonality – The Gram-Schmidt algorithm

1. Two vectors u and v are orthogonal if $(u, v) = 0$.
2. A system of vectors $\{v_1, \ldots, v_n\}$ is orthogonal if $(v_i, v_j) = 0$ for $i \neq j$; and orthonormal if $(v_i, v_j) = \delta_{ij}$
3. A matrix is orthogonal if its columns are orthonormal

➤ Notation: $V = [v_1, \ldots, v_n]$ == matrix with column-vectors $v_1, \ldots, v_n$.

Least-Squares systems

➤ Given: an $m \times n$ matrix $n < m$. Problem: find x which minimizes:

$$\|b - Ax\|_2$$

➤ Good illustration: Data fitting.

Typical problem of data fitting: We seek an unknwon function as a linear combination ϕ of n known functions ϕ_i (e.g. polynomials, trig. functions). Experimental data (not accurate) provides measures $\beta_1, \ldots, \beta_m$ of this unknown function at points $t_1, \ldots, t_m$. Problem: find the 'best' possible approximation ϕ to this data.

$$\phi(t) = \sum_{i=1}^{n} \xi_i \phi_i(t) \quad , \quad \text{s.t.} \quad \phi(t_j) \approx \beta_j, j = 1, \ldots, m$$

➤ Question: Close in what sense?

➤ Least-squares approximation: Find ϕ such that

$$\phi(t) = \sum_{i=1}^{n} \xi_i \phi_i(t), \;\; \& \;\; \sum_{j=1}^{m} |\phi(t_j) - \beta_j|^2 = \text{Min}$$

➤ In linear algebra terms: find 'best' approximation to a vector b from linear combinations of vectors f_i, $i = 1, \ldots, n$, where

$$b = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_m \end{pmatrix}, \quad f_i = \begin{pmatrix} \phi_i(t_1) \\ \phi_i(t_2) \\ \vdots \\ \phi_i(t_m) \end{pmatrix}$$

➤ We want to find $x = \{\xi_i\}_{i=1,\ldots,n}$ such that

$$\left\| \sum_{i=1}^{n} \xi_i f_i - b \right\|_2 \quad \text{Minimum}$$

Define

$$F = [f_1, f_2, \ldots, f_n], \quad x = \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_n \end{pmatrix}$$

➤ We want to find x to **minimize $\|b - Fx\|_2$**

➤ This is a Least-squares linear system: F is $m \times n$, with $m \geq n$.

✍ Formulate the least-squares system for the problem of finding the polynomial of degree 2 that approximates a function f which satisfies $\boxed{f(-1) = -1; f(0) = 1; f(1) = 2;\ f(2) = 0}$

Solution: $\phi_1(t) = 1; \quad \phi_2(t) = t; \quad \phi_2(t) = t^2$;

- Evaluate the ϕ_i's at points $t_1 = -1; t_2 = 0; t_3 = 1; t_4 = 2$:

$$f_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \quad f_2 = \begin{pmatrix} -1 \\ 0 \\ 1 \\ 2 \end{pmatrix} \quad f_3 = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 4 \end{pmatrix} \quad \to$$

➤ So the coefficients ξ_1, ξ_2, ξ_3 of the polynomial $\xi_1 + \xi_2 t + \xi_3 t^2$ are the solution of the least-squares problem $\min \|b - Fx\|$ where:

$$F = \begin{pmatrix} 1 & -1 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \end{pmatrix} \quad b = \begin{pmatrix} -1 \\ 1 \\ 2 \\ 0 \end{pmatrix}$$

THEOREM. The vector x_* mininizes $\psi(x) = \|b - Fx\|_2^2$ if and only if it is the solution of the normal equations:

$$F^T F x = F^T b$$

Proof: Expand out the formula for $\psi(x_* + \delta x)$:

$$\psi(x_* + \delta x) = ((b - Fx_*) - F\delta x)^T((b - Fx_*) - F\delta x)$$
$$= \psi(x_*) - 2(F\delta x)^T(b - Fx_*) + (F\delta x)^T(F\delta x)$$
$$= \psi(x_*) - 2(\delta x)^T \underbrace{\boxed{[F^T(b - Fx_*)]}}_{-\nabla_x \psi} + \underbrace{(F\delta x)^T(F\delta x)}_{\text{always positive}}$$

Can see that $\psi(x_* + \delta x) \geq \psi(x_*)$ for any δx, iff the boxed quantity [the gradient vector] is zero. Q.E.D.

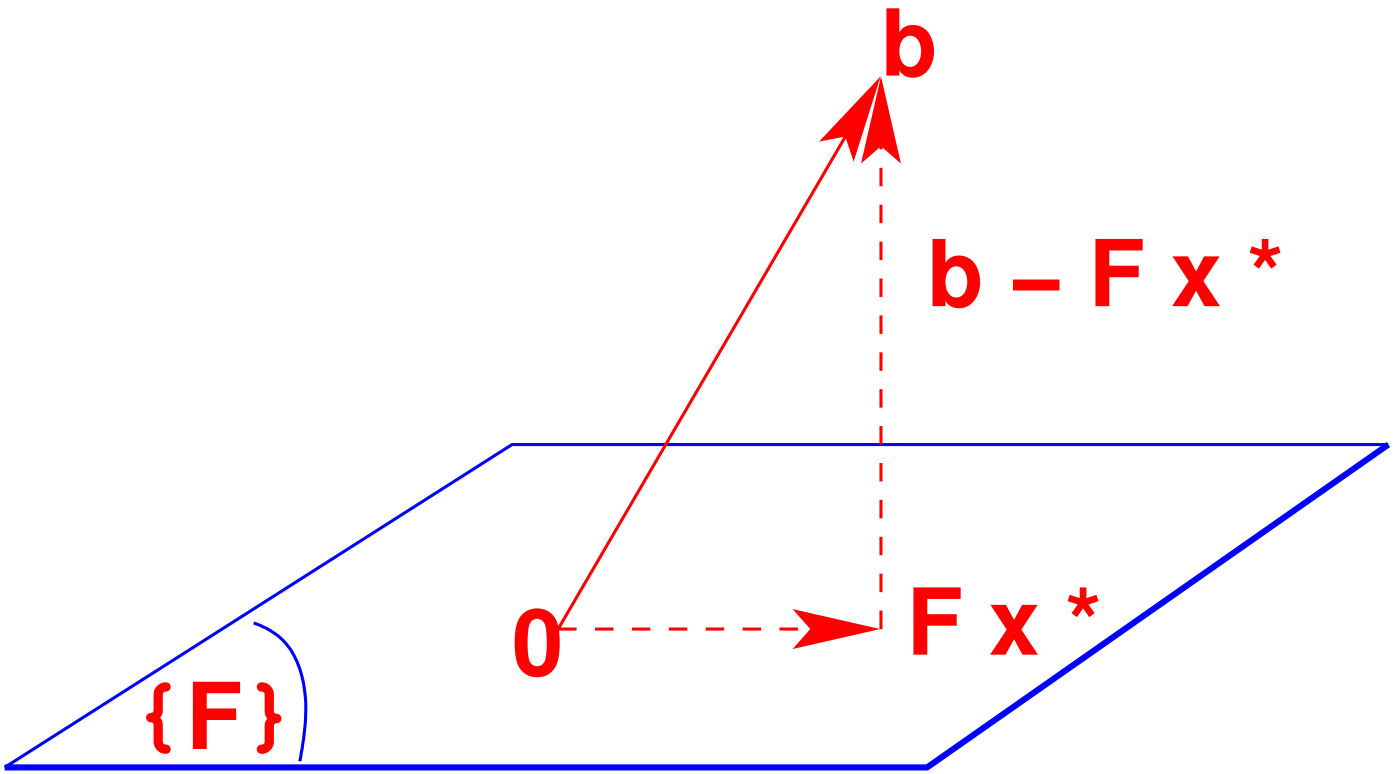
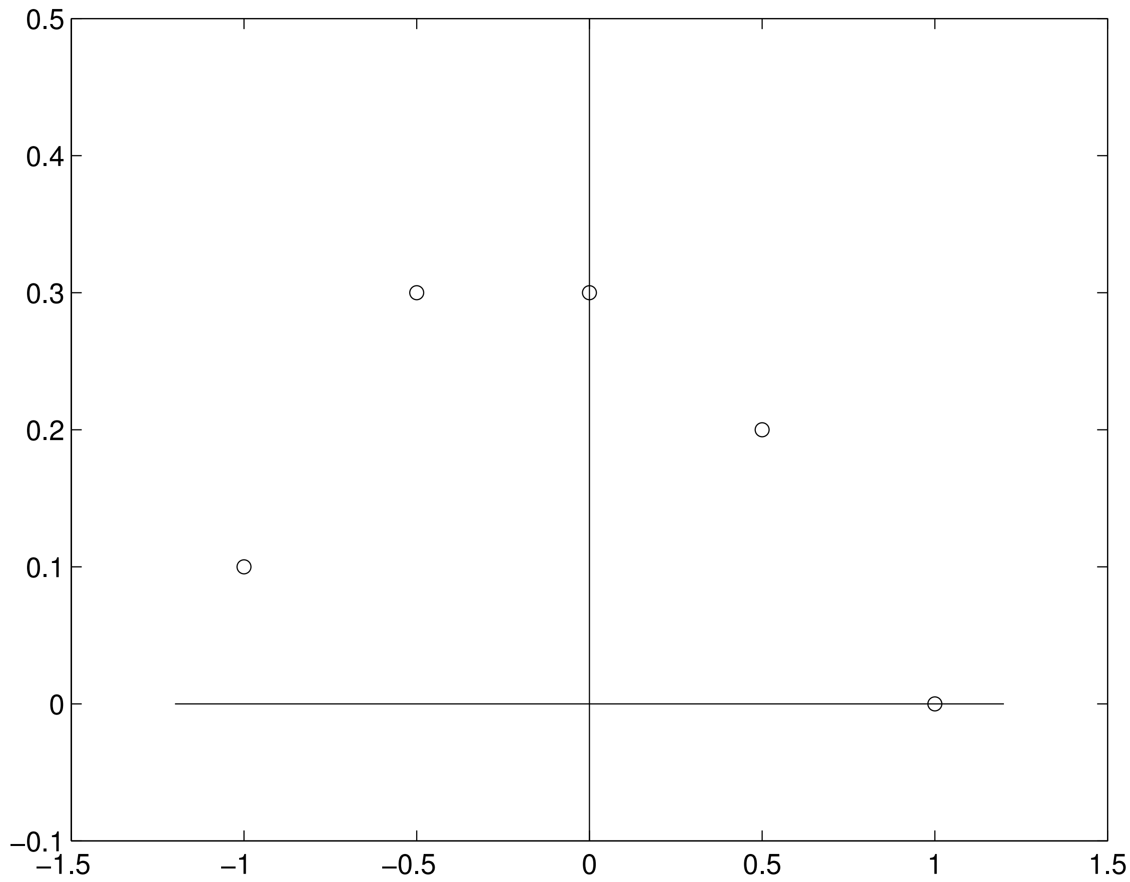


Illustration of theorem: x^* is the best approximation to the vector b from the subspace $\mathrm{span}\{F\}$ if and only if $b - Fx^*$ is $\perp$ to the whole subspace $\mathrm{span}\{F\}$. This in turn is equivalent to $F^T(b - Fx^*) = 0$ ➤ Normal equations.

Example:

Points:	$t_1 = -1$	$t_2 = -1/2$	$t_3 = 0$	$t_4 = 1/2$	$t_5 = 1$
Values:	$\beta_1 = 0.1$	$\beta_2 = 0.3$	$\beta_3 = 0.3$	$\beta_4 = 0.2$	$\beta_5 = 0.0$



1) Approximations by polynomials of degree one:

- $\phi_1(t) = 1, \phi_2(t) = t.$

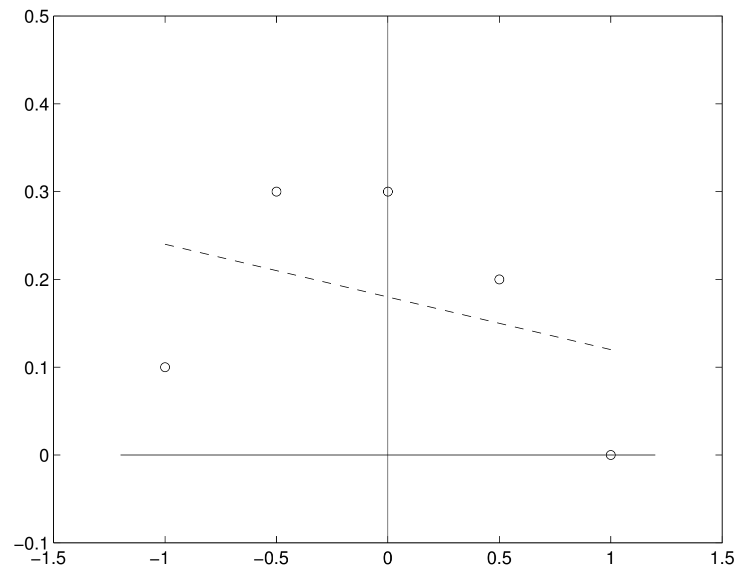
$$F = \begin{pmatrix} 1.0 & -1.0 \\ 1.0 & -0.5 \\ 1.0 & 0 \\ 1.0 & 0.5 \\ 1.0 & 1.0 \end{pmatrix}$$

$$F^T F = \begin{pmatrix} 5.0 & 0 \\ 0 & 2.5 \end{pmatrix}$$

$$F^T b = \begin{pmatrix} 0.9 \\ -0.15 \end{pmatrix}$$

- Best approximation is

$$\boxed{\phi(t) = 0.18 - 0.06t}.$$

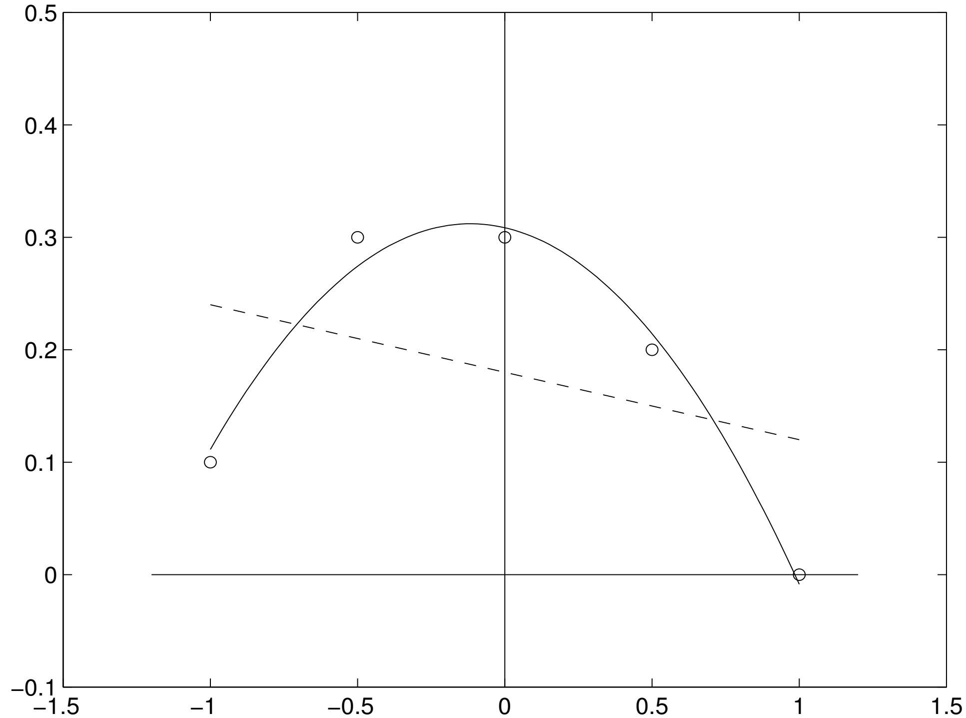


TB: 7,8,11,19; AB: 2.1, 2.3.4, ;GvL 5, 5.3 – QR

2) Approximation by polynomials of degree 2:

- $\phi_1(t) = 1, \phi_2(t) = t, \phi_3(t) = t^2$.
- Best polynomial found:

$$0.3085714285 - 0.06 \;\times t \; - 0.2571428571 \;\times t^2$$



Problem with Normal Equations

- Condition number is high: if A is square and non-singular, then

$$\kappa_2(A) = \|A\|_2 \cdot \|A^{-1}\|_2 = \sigma_{\max}/\sigma_{\min}$$
$$\kappa_2(A^T A) = \|A^T A\|_2 \cdot \|(A^T A)^{-1}\|_2 = (\sigma_{\max}/\sigma_{\min})^2$$

- Example: Let $A = \begin{pmatrix} 1 & 1 & -\epsilon \\ \epsilon & 0 & 1 \\ 0 & \epsilon & 1 \end{pmatrix}$.

- Then $\kappa(A) \approx \sqrt{2}/\epsilon$, but $\kappa(A^T A) \approx 2\epsilon^{-2}$.

- $$fl(A^T A) = fl \begin{pmatrix} 2 + \epsilon^2 & 1 & 0 \\ 1 & 1 + \epsilon^2 & 0 \\ 0 & 0 & 1 + \epsilon^2 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

is singular to working precision (if $\epsilon < \underline{\mathbf{u}}$).

Finding an orthonormal basis of a subspace

- Goal: Find vector in $\mathbf{span}(X)$ closest to b.
- Much easier with an orthonormal basis for $\mathbf{span}(X)$.

Problem: Given $X = [x_1, \ldots, x_n]$, compute $Q = [q_1, \ldots, q_n]$ which has orthonormal columns and s.t. $\mathbf{span}(Q) = \mathbf{span}(X)$

- Note: each column of X must be a linear combination of certain columns of Q.
- We will find Q so that x_j (j column of X) is a linear combination of the first j columns of Q.

ALGORITHM : 1. *Classical Gram-Schmidt*

1. *For* $j = 1, \ldots, n$ *Do:*
2. *Set* $\hat{q} := x_j$
3. *Compute* $r_{ij} := (\hat{q}, q_i)$, *for* $i = 1, \ldots, j-1$
4. *For* $i = 1, \ldots, j-1$ *Do :*
5. *Compute* $\hat{q} := \hat{q} - r_{ij} q_i$
6. *EndDo*
7. *Compute* $r_{jj} := \|\hat{q}\|_2$,
8. *If* $r_{jj} = 0$ *then Stop, else* $q_j := \hat{q}/r_{jj}$
9. *EndDo*

➤ All n steps can be completed iff $x_1, x_2, \ldots, x_n$ are linearly independent.

➤ Lines 5 and 7-8 show that

$$x_j = r_{1j}q_1 + r_{2j}q_2 + \ldots + r_{jj}q_j$$

➤ If $X = [x_1, x_2, \ldots, x_n]$, $Q = [q_1, q_2, \ldots, q_n]$, and if R is the $n \times n$ upper triangular matrix

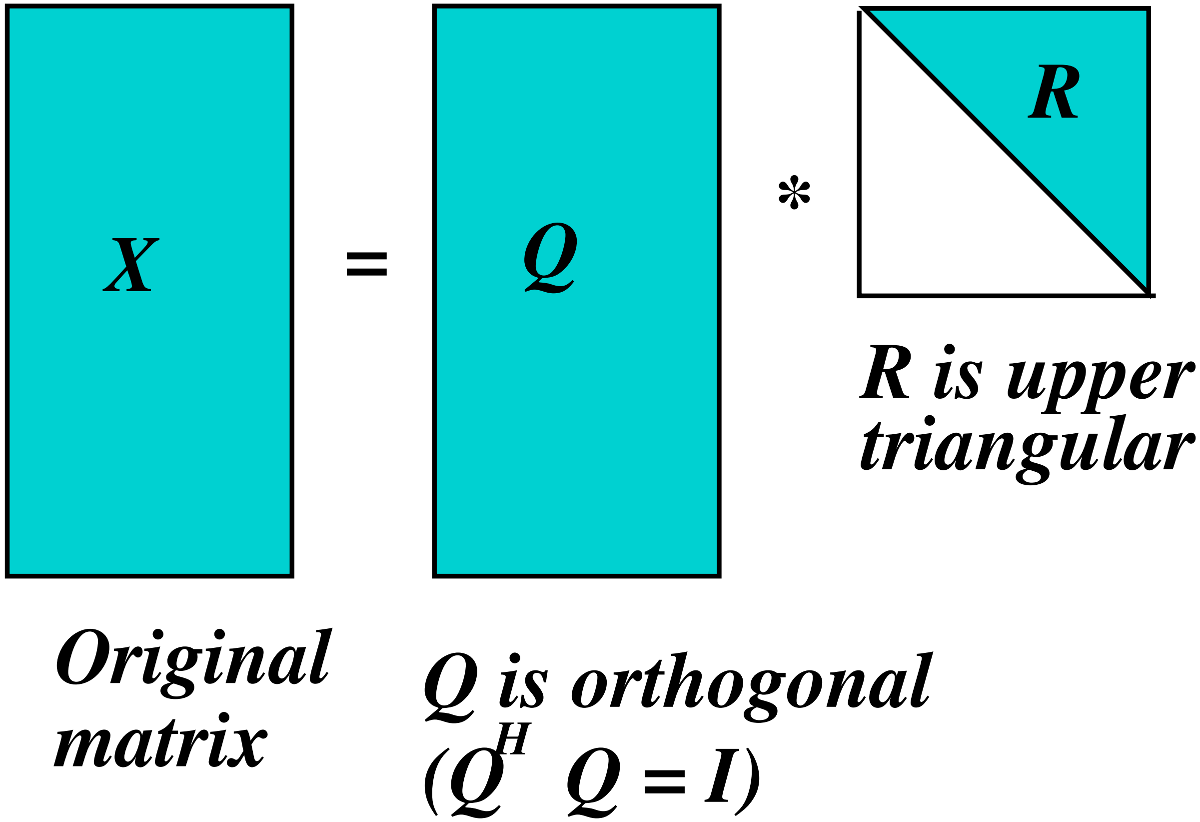
$$R = \{r_{ij}\}_{i,j=1,\ldots,n}$$

then the above relation can be written as

$$X = QR$$

➤ R is upper triangular, Q is orthogonal. This is called the *QR factorization* of X.

✍ What is the cost of the factorization when $X \in \mathbb{R}^{m\times n}$?



Another decomposition:

A matrix X, with linearly independent columns, is the product of an orthogonal matrix Q and a upper triangular matrix R.

➤ Better algorithm: Modified Gram-Schmidt.

ALGORITHM : 2. *Modified Gram-Schmidt*

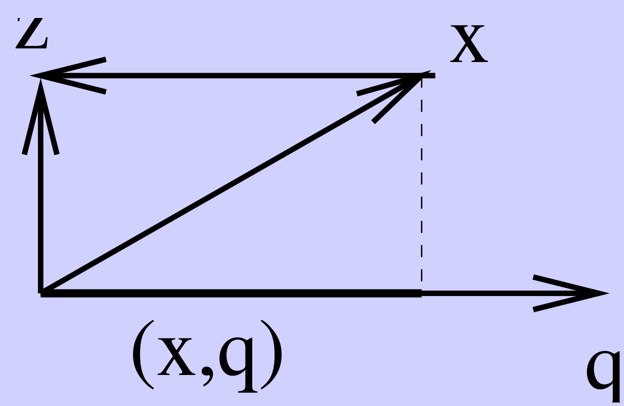
1. For $j = 1, \ldots, n$ Do:
2. Define $\hat{q} := x_j$
3. For $i = 1, \ldots, j-1$, Do:
4. $r_{ij} := (\hat{q}, q_i)$
5. $\hat{q} := \hat{q} - r_{ij} q_i$
6. EndDo
7. Compute $r_{jj} := \|\hat{q}\|_2$,
8. If $r_{jj} = 0$ then Stop, else $q_j := \hat{q}/r_{jj}$
9. EndDo

Only difference: inner product uses the accumulated subsum instead of original $\hat{q}$

The operations in lines 4 and 5 can be written as

$$\hat{q} := \boldsymbol{ORTH}(\hat{q}, q_i)$$

where $\boldsymbol{ORTH(x, q)}$ denotes the operation of orthogonalizing a vector $\boldsymbol{x}$ against a unit vector $\boldsymbol{q}$.



Result of $\boldsymbol{z = ORTH(x, q)}$

➤ Modified Gram-Schmidt algorithm is much more stable than classical Gram-Schmidt in general. [A few examples easily show this].

Suppose MGS is applied to A yielding computed matrices $\hat{Q}$ and $\hat{R}$. Then there are constants c_i (depending on (m, n)) such that

$$A + E_1 = \hat{Q}\hat{R} \qquad \|E_1\|_2 \le c_1 \, \underline{\mathbf{u}} \, \|A\|_2$$

$$\|\hat{Q}^T\hat{Q} - I\|_2 \le c_2 \, \underline{\mathbf{u}} \, \kappa_2(A) + O((\underline{\mathbf{u}} \, \kappa_2(A))^2)$$

for a certain perturbation matrix E_1, and there exists an orthonormal matrix Q such that

$$A + E_2 = Q\hat{R} \qquad \|E_2(:, j)\|_2 \le c_3 \underline{\mathbf{u}} \, \|A(:, j)\|_2$$

for a certain perturbation matrix E_2.

➤ An equivalent version:

ALGORITHM : 3. *Modified Gram-Schmidt - 2 -*

0. Set $\hat{Q} := X$
1. For $i = 1, \ldots, n$ Do:
2. Compute $r_{ii} := \|\hat{q}_i\|_2$,
3. If $r_{ii} = 0$ then Stop, else $q_i := \hat{q}_i / r_{ii}$
4. For $j = i + 1, \ldots, n$, Do:
5. $r_{ij} := (\hat{q}_j, q_i)$
6. $\hat{q}_j := \hat{q}_j - r_{ij} q_i$
7. EndDo
8. EndDo

➤ Does exactly the same computation as previous algorithm, but in a different order.

Example:

Orthonormalize the system of vectors:

$$X = [x_1, x_2, x_3] = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & -1 \\ 1 & 0 & 4 \end{pmatrix}$$

Answer:

$$q_1 = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \quad ; \quad \hat{q}_2 = x_2 - (x_2, q_1) q_1 = \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} - 1 \times \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$$

$$\hat{q}_2 = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ -\frac{1}{2} \\ -\frac{1}{2} \end{pmatrix} ; \quad q_2 = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ -\frac{1}{2} \\ -\frac{1}{2} \end{pmatrix}$$

$$\hat{q}_3 = x_3 - (x_3, q_1)q_1 = \begin{pmatrix} 1 \\ 0 \\ -1 \\ 4 \end{pmatrix} - 2 \times \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \\ -2 \\ 3 \end{pmatrix}$$

$$\hat{q}_3 = \hat{q}_3 - (\hat{q}_3, q_2)q_2 = \begin{pmatrix} 0 \\ -1 \\ -2 \\ 3 \end{pmatrix} - (-1) \times \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ -\frac{1}{2} \\ -\frac{1}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ -2.5 \\ 2.5 \end{pmatrix}$$

$$\|\hat{q}_3\|_2 = \sqrt{13} \rightarrow q_3 = \frac{\hat{q}_3}{\|\hat{q}_3\|_2} = \frac{1}{\sqrt{13}} \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ -2.5 \\ 2.5 \end{pmatrix}$$

✍ For this example: what is Q? what is R? Compute Q^TQ.

➤ Result is the identity matrix.

Recall: For any orthogonal matrix Q, we have

$$Q^TQ = I$$

(In complex case: $Q^HQ = I$).
Consequence: For an $n \times n$ orthogonal matrix $\boxed{Q^{-1} = Q^T}$.
(Q is orthogonal/ unitary)

Application: another method for solving linear systems.

$$Ax = b$$

A is an $n \times n$ nonsingular matrix. Compute its QR factorization.

- Multiply both sides by $Q^T \rightarrow Q^T QRx = Q^T b \rightarrow$

$$Rx = Q^T b$$

Method:

- Compute the QR factorization of A, $A = QR$.
- Solve the upper triangular system $Rx = Q^T b$.

✍ Cost??

Use of the QR factorization

Problem: $Ax \approx b$ in least-squares sense

A is an $m \times n$ (full-rank) matrix. Let

$$A = QR$$

the QR factorization of A and consider the normal equations:

$$A^T A x = A^T b \;\rightarrow\; R^T Q^T Q R x = R^T Q^T b \;\rightarrow$$

$$R^T R x = R^T Q^T b \rightarrow R x = Q^T b$$

(R^T is an $n \times n$ nonsingular matrix). Therefore,

$$x = R^{-1} Q^T b$$

Another derivation:

- Recall: $\mathbf{span}(Q) = \mathbf{span}(A)$
- So $\|b - Ax\|_2$ is minimum when $b - Ax \perp \mathbf{span}\{Q\}$
- Therefore solution x must satisfy $Q^T(b - Ax) = 0 \rightarrow$

$$Q^T(b - QRx) = 0 \rightarrow Rx = Q^T b$$

$$x = R^{-1}Q^T b$$

- Also observe that for any vector w

$$w = QQ^T w + (I - QQ^T)w$$

and that $w = QQ^T w \quad \perp \quad (I - QQ^T)w \ \rightarrow$

- Pythagoras theorem $\longrightarrow$ $\|w\|_2^2 = \|QQ^T w\|_2^2 + \|(I - QQ^T)w\|_2^2$

$$\begin{aligned}\|b - Ax\|^2 &= \|b - QRx\|^2 \\ &= \|(I - QQ^T)b + Q(Q^T b - Rx)\|^2 \\ &= \|(I - QQ^T)b\|^2 + \|Q(Q^T b - Rx)\|^2 \\ &= \|(I - QQ^T)b\|^2 + \|Q^T b - Rx\|^2\end{aligned}$$

- Min is reached when 2nd term of r.h.s. is zero.

Method:

- Compute the QR factorization of A, $A = QR$.
- Compute the right-hand side $f = Q^T b$
- Solve the upper triangular system $Rx = f$.
- x is the least-squares solution

➤ As a rule it is not a good idea to form $A^T A$ and solve the normal equations. Methods using the QR factorization are better.

✍ Total cost?? (depends on the algorithm used to get the QR decomposition).

✍ Using matlab find the parabola that fits the data in previous data fitting example (p. 8-10) in L.S. sense [verify that the result found is correct.]