The QR factorization and Least-Squares Systems

- Orthogonality
- The Gram-Schmidt and Modified Gram-Schmidt processes. Text: 5.2.7 , 5.2.8
- Least-squares systems. Text: 5.3
- The Householder QR and the Givens QR. Text: 5.1 , 5.2 .

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 $v_1, \ldots, v_n$.

IMPORTANT: From now on, we will reserve the term unitary for square matrices. The term 'orthonormal matrix' is not used. Even 'orthogonal' is often used for square matrices.

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

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

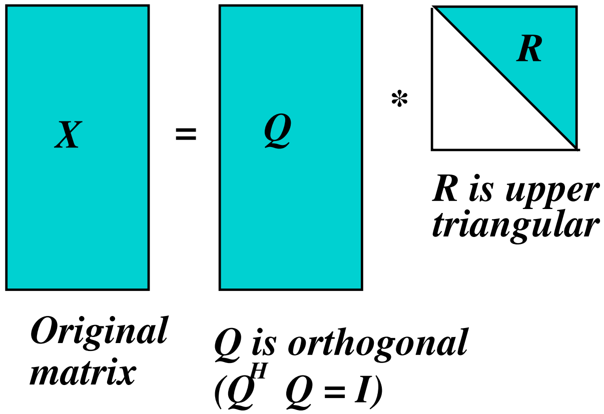
$$R = \{r_{ij}\}_{i,j=1,\ldots,n}$$

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**

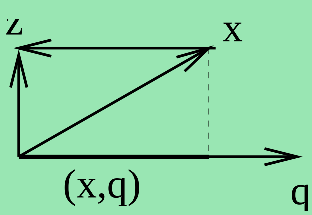
1. For $j = 1, \ldots, n$ Do:
2. Define $\hat{q} := x_j$
3. For $i = 1, \ldots, j-1$, Do:
4. $r_{ij} := (\hat{q}, q_i)$
5. $\hat{q} := \hat{q} - r_{ij} q_i$
6. EndDo
7. Compute $r_{jj} := \|\hat{q}\|_2$,
8. If $r_{jj} = 0$ then Stop, else $q_j := \hat{q}/r_{jj}$
9. EndDo

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

The operations in lines 4 and 5 can be written as

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

Where $ORTH(x, q)$ denotes the operation of orthogonalizing a vector x against a unit vector q.



Result of $z = ORTH(x, q)$

➤ **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

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

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

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

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

for a certain perturbation matrix E_2.

➤ **An equivalent version:**

ALGORITHM : 3. Modified Gram-Schmidt - 2 -

1. For $j = 1, \ldots, n$ Do:
2. $\quad$ Compute $r_{jj} := \|\hat{x}_j\|_2$,
3. $\quad$ If $r_{jj} = 0$ then Stop, else $q_j := \hat{x}_j / r_{jj}$
4. $\quad$ For $i = j+1, \ldots, n$, Do:
5. $\quad\quad r_{ji} := (x_i, q_j)$
6. $\quad\quad x_i := x_i - r_{ji} q_j$
7. $\quad$ 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:

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

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

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

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

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

For this example: compute $Q^T Q$.

➤ **Result is the identity matrix.**

Recall: For any orthogonal matrix Q, we have

$$\boxed{Q^T Q = I}$$

(In complex case: $Q^H Q = I$).

Consequence: For an $n \times n$ orthogonal matrix $\boxed{Q^{-1} = Q^T}$. (Q is 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 $Q^T \to Q^TQRx = Q^Tb \to$

$$Rx = Q^Tb$$

Method:

➤ Compute the QR factorization of A, $A = QR$.

➤ Solve the upper triangular system $Rx = Q^Tb$.

Cost??

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.

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

➤ Question: Close in what sense?

➤ Least-squares approximation: Find ϕ such that

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

➤ Translated in linear algebra terms: find 'best' approximation vector 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 $\boxed{\|b - Fx\|_2}$.

➤ Least-squares linear system. F is $m \times n$, with $m > n$.

THEOREM. The vector x_* mininizes $\|b - Fx\|_2$ if and only if it is the solution of the normal equations:

$$F^TFx = F^Tb$$

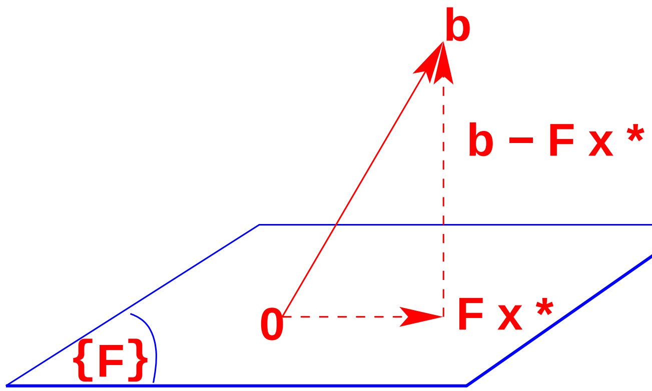
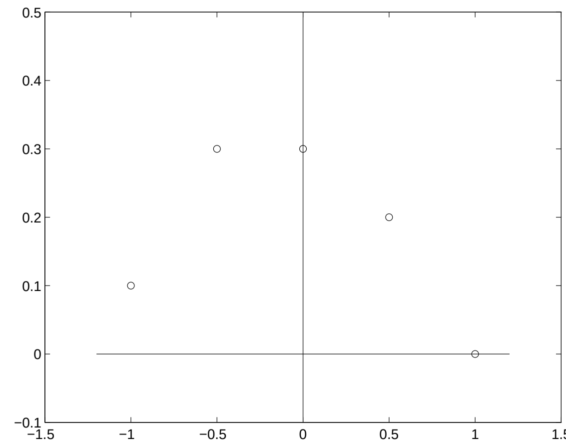


Illustration of theorem: x^* is the best approximation to the vector b from the subspace $\mathrm{span}\{F\}$ if and only if $b - Fx^*$ is $\perp$ to the whole subspace $\mathrm{span}\{F\}$. This in turn is equivalent to $F^T(b - Fx^*) = 0$ ➤ Normal equations.

Example:

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

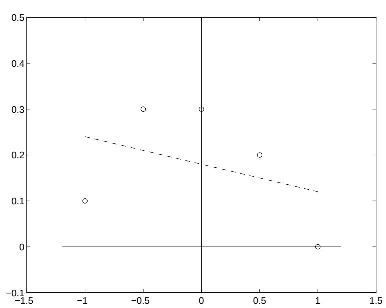


1) Approximations by polynomials of degree one:

➤ $\phi_1(t) = 1, \phi_2(t) = t.$

$$F = \begin{pmatrix} 1.0 & -1.0 \\ 1.0 & -0.5 \\ 1.0 & 0 \\ 1.0 & 0.5 \\ 1.0 & 1.0 \end{pmatrix} \qquad F^TF = \begin{pmatrix} 5.0 & 0 \\ 0 & 2.5 \end{pmatrix} \quad F^Tb = \begin{pmatrix} 0.9 \\ -0.15 \end{pmatrix}$$

➤ **Best approximation is** $\boxed{\phi(t) = 0.18 - 0.06t}$.

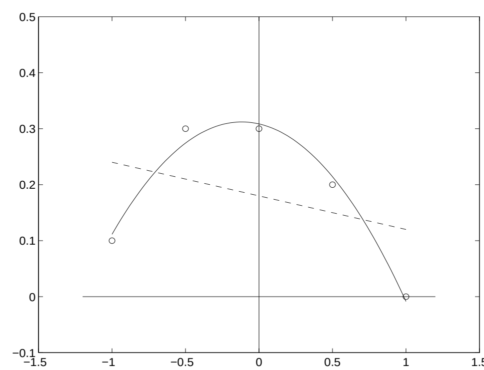


2) Approximation by polynomials of degree 2:

➤ $\phi_1(t) = 1, \phi_2(t) = t, \phi_3(t) = t^2.$

➤ **Best polynomial found:**

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



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:

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

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

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

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

Another derivation:

- Recall: $\mathrm{span}(Q) = \mathrm{span}(X)$
- So $\|b - Ax\|_2$ is minimum when $b - Ax \perp \mathrm{span}\{Q\}$
- 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:

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

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

- 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??

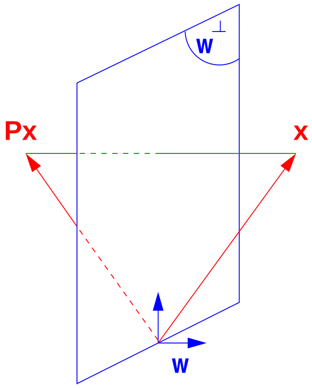
✍ Using matlab find the parabola that fits the data in previous example in L.S. sense [verify that the result found is correct.]

Householder QR

➤ Householder reflectors are matrices of the form

$$P = I - 2ww^T,$$

where w is a unit vector (a vector of 2-norm unity)



Geometrically, Px represents a mirror image of x with respect to the hyperplane $\mathrm{span}\{w\}^\perp$.

A few simple properties:

- P is symmetric (real for w real) – It is also unitary (for real w)
- In the complex case $P = I - 2ww^H$ is Hermitian and unitary.
- P can be written as $P = I - \beta vv^T$ with $\beta = 2/\|v\|_2^2$, where v is a multiple of w. [storage: v and β]
- Px can be evaluated $x - \beta(x^T v) \times v$ (op count?)
- Similarly: $PA = A - vz^T$ where $z^T = \beta * v^T * A$

➤ NOTE: we work in $\mathbb{R}^m$, so all vectors are of length m, P is of size $m \times m$, etc.

Problem 1: Given a vector $x \neq 0$, find w such that

$$(I - 2ww^T)x = \alpha e_1,$$

where α is a (free) scalar.

Writing $(I - \beta vv^T)x = \alpha e_1$ yields

$$\beta(v^T x)\ v = x - \alpha e_1. \qquad (1)$$

➤ Desired w is a multiple of $x - \alpha e_1$, i.e., we can take

$$v = x - \alpha e_1$$

➤ To determine α we just recall that

$$\|(I - 2ww^T)x\|_2 = \|x\|_2$$

➤ As a result: $|\alpha| = \|x\|_2$, or

$$\alpha = \pm\|x\|_2$$

➤ Should verify that both signs work, i.e., that in both cases we indeed get $Px = \alpha e_1$ [exercise]

➤ Which sign is best? To reduce cancellation, the resulting $x - \alpha e_1$ should not be small. So, $\alpha = -\mathrm{sign}(\xi_1)\|x\|_2$.

$$v = x + \mathrm{sign}(\xi_1)\|x\|_2 e_1 \text{ and } \beta = 2/\|v\|_2^2$$

$$v = \begin{pmatrix} \hat{\xi}_1 \\ \xi_2 \\ \vdots \\ \xi_{m-1} \\ \xi_m \end{pmatrix} \quad \text{with} \quad \hat{\xi}_1 = \begin{cases} \xi_1 + \|x\|_2 & \text{if } \xi_1 > 0 \\ \xi_1 - \|x\|_2 & \text{if } \xi_1 \leq 0 \end{cases}$$

➤ OK, but will yield a negative multiple of e_1 if $\xi_1 > 0$.

.. Show that $(I - \beta vv^T)x = \alpha e_1$ when $v = x - \alpha e_1$ and $\alpha = \pm\|x\|_2$.

- Equivalent to showing that

$$x - (\beta x^T v)v = \alpha e_1 \leftrightarrow x - \alpha e_1 = (\beta x^T v)v$$

but recall that $v = x - \alpha e_1$ so we need to show that

$$\beta x^T v = 1 \quad \text{i.e., that} \quad \frac{2x^T v}{\|x - \alpha e_1\|_2^2} = 1$$

- Denominator $= \|x\|_2^2 + \alpha^2 - 2\alpha e_1^T x = 2(\|x\|_2^2 - \alpha e_1^T x)$
- Numerator $= 2x^T v = 2x^T(x - \alpha e_1) = 2(\|x\|_2^2 - \alpha x^T e_1)$

Numerator/ Denominator = 1. Done

Alternative:

- Define $\sigma = \sum_{i=2}^m \xi_i^2$.
- Always set $\hat{\xi}_1 = \xi_1 - \|x\|_2$. Update OK when $\xi_1 \le 0$
- When $\xi_1 > 0$ compute $\hat{x}_1$ as

$$\hat{\xi}_1 = \xi_1 - \|x\|_2 = \frac{\xi_1^2 - \|x\|_2^2}{\xi_1 + \|x\|_2} = \frac{-\sigma}{\xi_1 + \|x\|_2}$$

So: $$\hat{\xi}_1 = \begin{cases} \frac{-\sigma}{\xi_1 + \|x\|_2} & \text{if } \xi_1 > 0 \\ \xi_1 - \|x\|_2 & \text{if } \xi_1 \le 0 \end{cases}$$

- It is customary to compute a vector v such that $v_1 = 1$. So v is scaled by its first component.
- If σ is zero, procedure will return $v = [1; x(2:m)]$ and $\beta = 0$.
- Matlab function:

```
function [v,bet] = house (x)
%% computes the householder vector for x
m = length(x);
v = [1 ; x(2:m)];
sigma = v(2:m)' * v(2:m);
if (sigma == 0)
   bet = 0;
else
   xnrm = sqrt(x(1)^2 + sigma) ;
   if (x(1) <= 0)
      v(1) = x(1) - xnrm;
   else
      v(1) = -sigma / (x(1) + xnrm) ;
   end
   bet = 2 / (1+sigma/v(1)^2);
   v = v/v(1) ;
end
```


Problem 2: Generalization.

Given an $m \times n$ matrix X, find $w_1, w_2, \ldots, w_n$ such that

$$(I - 2w_n w_n^T) \cdots (I - 2w_2 w_2^T)(I - 2w_1 w_1^T)X = R$$

where $r_{ij} = 0$ for $i > j$

- First step is easy : select w_1 so that the first column of X becomes αe_1
- Second step: select w_2 so that x_2 has zeros below 2nd component.
- etc.. After $k-1$ steps: $X_k \equiv P_{k-1} \ldots P_1 X$ has the following shape:

$$X_k = \begin{pmatrix} x_{11} & x_{12} & x_{13} & \cdots & \cdots & \cdots & x_{1n} \\ & x_{22} & x_{23} & \cdots & \cdots & \cdots & x_{2n} \\ & & x_{33} & \cdots & \cdots & \cdots & x_{3n} \\ & & & \ddots & \cdots & \cdots & \vdots \\ & & & & x_{kk} & \cdots & \vdots \\ & & & & x_{k+1,k} & \cdots & x_{k+1,n} \\ & & & & \vdots & \vdots & \vdots \\ & & & & x_{m,k} & \cdots & x_{m,n} \end{pmatrix}.$$

➤ To do: transform this matrix into one which is upper triangular up to the k-th column...

➤ ... while leaving the previous columns untouched.

➤ To leave the first $k-1$ columns unchanged w must have zeros in positions 1 through $k-1$.

$$P_k = I - 2w_k w_k^T, \quad w_k = \frac{v}{\|v\|_2},$$

where the vector v can be expressed as a Householder vector for a shorter vector using the matlab function house,

$$v = \begin{pmatrix} 0 \\ house(X(k:m,k)) \end{pmatrix}$$

➤ The result is that work is done on the $(k:m, k:n)$ submatrix.

ALGORITHM : 4. Householder QR

1. For $k = 1:n$ do
2. $\quad [v, \beta] = house(X(k:m,k))$
3. $\quad X(k:m,k:n) = (I - \beta vv^T)X(k:m,k:n)$
4. $\quad$ If $(k < m)$
5. $\quad\quad X(k+1:m,k) = v(2:m-k+1)$
6. $\quad$ end
7. end

➤ In the end:

$$X_n = P_n P_{n-1} \dots P_1 X = \text{upper triangular}$$

Yields the factorization:

$$X = QR$$

where

$$Q = P_1 P_2 \dots P_n \text{ and } R = X_n$$

MAJOR difference with Gram-Schmidt: Q is $m \times m$ and R is $m \times n$ (same as X). The matrix R has zeros below the n-th row. Note also : this factorization always exists.

Cost of Householder QR? Compare with Gram-Schmidt

Question: How to obtain $X = Q_1 R_1$ where Q_1 = same size as X and R_1 is $n \times n$ (as in MGS)?

Answer: simply use the partitioning

$$X = \begin{pmatrix} Q_1 & Q_2 \end{pmatrix} \begin{pmatrix} R_1 \\ 0 \end{pmatrix} \quad \rightarrow \quad X = Q_1 R_1$$

➤ Referred to as the "thin" QR factorization (or "economy-size QR" factorization in matlab)

➤ How to solve a least-squares problem $Ax = b$ using the Householder factorization?

➤ Answer: no need to compute Q_1. Just apply Q^T to b.

➤ This entails applying the successive Householder reflections to b

The rank-deficient case

➤ Result of Householder QR: Q_1 and R_1 such that $Q_1 R_1 = X$. In the rank-deficient case, can have $\text{span}\{Q_1\} \neq \text{span}\{X\}$ because R_1 may be singular.

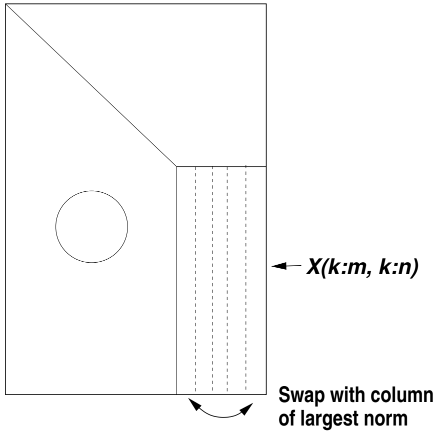
➤ Remedy: Householder QR with column pivoting. Result will be:

$$A\Pi = Q \begin{pmatrix} R_{11} & R_{12} \\ 0 & 0 \end{pmatrix}$$

➤ R_{11} is nonsingular. So rank(X) = size of R_{11} = rank(Q_1) and Q_1 and X span the same subspace.

➤ Π permutes columns of X.

Algorithm: At step k, active matrix is $X(k:m, k:n)$. Swap k-th column with column of largest 2-norm in $X(k:m, k:n)$. If all the columns have zero norm, stop.



Practical Question: how to implement this ???

Properties of the QR factorization

Consider the 'thin' factorization $A = QR$, (size(Q) = [m,n] = size (A)). Assume $r_{ii} > 0$, $i = 1, \ldots, n$

1. When A is of full column rank this factorization exists and is unique

2. It satisfies:

$$\text{span}\{a_1, \cdots, a_k\} = \text{span}\{q_1, \cdots, q_k\}, \quad k = 1, \ldots, n$$

3. R is identical with the Cholesky factor G^T of $A^T A$.

➤ When A in rank-deficient and Householder with pivoting is used, then

$$Ran\{Q_1\} = Ran\{A\}$$

Givens Rotations

- Matrices of the form

$$G(i,k,\theta) = \begin{array}{c} \begin{pmatrix} 1 & \dots & 0 & & \dots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & c & \dots & s & \dots & 0 \\ \vdots & \dots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & \dots & -s & \dots & c & \dots & 0 \\ \vdots & \dots & \vdots & \dots & \vdots & \dots & \vdots \\ 0 & \dots & 0 & & \dots & & 1 \end{pmatrix} \end{array} \begin{array}{c} \\ \\ i \\ \\ k \\ \\ \\ \end{array}$$

with $c = \cos\theta$ and $s = \sin\theta$

- represents a rotation in the span of e_i and e_k.

Main idea of Givens rotations consider $y = Gx$ then

$$\begin{aligned} y_i &= c * x_i + s * x_k \\ y_k &= -s * x_i + c * x_k \\ y_j &= x_j \quad \text{for} \quad j \neq i, k \end{aligned}$$

- Can make $y_k = 0$ by selecting

$$s = x_k/t; \quad c = x_i/t; \quad t = \sqrt{x_i^2 + x_k^2}$$

- This is used to introduce zeros in the first column of a matrix A (for example $G(m-1,m)$, $G(m-2,m-1)$ etc..$G(1,2)$)..
- See text for details

Orthogonal projectors and subspaces

Notation: Given a supspace $\mathcal{X}$ or $\mathbb{R}^m$ define

$$\mathcal{X}^\perp = \{y \mid y \perp x, \quad \forall\, x \in \mathcal{X}\}$$

- Let $Q = [q_1, \cdots, q_r]$ an orthonormal basis of $\mathcal{X}$
- How would you obtain such a basis?
- Then define orthogonal projector $P = QQ^T$

Properties

(a) $P^2 = P$ (b) $(I-P)^2 = I - P$
(c) $Ran(P) = \mathcal{X}$ (d) $Ran(I-P) = Null(P)$
(e) $Null(P) = \mathcal{X}^\perp$ $(= Ran(I-P))$

- Note that (b) means that $I - P$ is also a projector

Proof. (a), (b) are trivial

(c): Clearly $Ran(P) = \{x \mid x = QQ^Ty, y \in \mathbb{R}^m\} \subseteq \mathcal{X}$. Any $x \in \mathcal{X}$ is of the form $x = Qy, y \in \mathbb{R}^m$. Take $Px = QQ^T(Qy) = Qy = x$. Since $x = Px$, $x \in Ran(P)$ so $\mathcal{X} \subseteq Ran(P)$. In the end $\mathcal{X} = Ran(P)$.

(d): Need to show inclusion both ways.

- $x \in Null(P) \leftrightarrow Px = 0 \leftrightarrow (I-P)x = x \rightarrow x \in Ran(I-P)$
- $x \in Ran(I-P) \leftrightarrow \exists y \in \mathbb{R}^m | x = (I-P)y \rightarrow Px = P(I-P)y = 0 \rightarrow x \in Null(P)$

(e): $x \in \mathcal{X}^\perp \leftrightarrow (x,y) = 0, \forall y \in \mathcal{X} \leftrightarrow (x, Qz) = 0, \forall z \in \mathbb{R}^r \leftrightarrow (Q^Tx, z) = 0, \forall z \in \mathbb{R}^r \leftrightarrow Q^Tx = 0 \leftrightarrow QQ^Tx = 0 \leftrightarrow Px = 0$

Orthogonal decomposition

Result: Any $x \in \mathbb{R}^m$ can be written in a unique way as

$$x = x_1 + x_2, \quad x_1 \in \mathcal{X}, \quad x_2 \in \mathcal{X}^\perp$$

- Just set $x_1 = Px, \quad x_2 = (I - P)x$
- In other words $\mathbb{R}^m = P\mathbb{R}^m \oplus (I-P)\mathbb{R}^m$ or
$$\mathbb{R}^m = Ran(P) \oplus Ran(I-P)$$
$$\mathbb{R}^m = Ran(P) \oplus Null(P)$$
- Can complete basis $\{q_1, \cdots, q_r\}$ into orthonormal basis of $\mathbb{R}^m$, $q_{r+1}, \cdots, q_m$
- $\{q_{r+1}, q_{r+2}, \cdots, q_m\}$ = basis of $\mathcal{X}^\perp$. $\rightarrow$
$$dim(\mathcal{X}^\perp) = m - r.$$

Four fundamental supspaces - URV decomposition

Let $A \in \mathbb{R}^{m\times n}$ and consider $\mathrm{Ran}(A)^\perp$

Property 1: $\mathrm{Ran}(A)^\perp = Null(A^T)$

Proof: $x \in \mathrm{Ran}(A)^\perp$ iff $(Ay, x) = 0$ for all y iff $(y, A^Tx) = 0$ for all y ...

Property 2: $\mathrm{Ran}(A^T) = Null(A)^\perp$

- Take $\mathcal{X} = \mathrm{Ran}(A)$ in orthogonal decomoposition
- Result:

$$\mathbb{R}^m = Ran(A) \oplus Null(A^T)$$
$$\mathbb{R}^n = Ran(A^T) \oplus Null(A)$$

4 fundamental subspaces

$Ran(A)$ $\quad Null(A)$,
$Ran(A^T)$ $\quad Null(A^T)$

- Express the above with bases for $\mathbb{R}^m$:

$$[\underbrace{u_1, u_2, \cdots, u_r}_{Ran(A)}, \underbrace{u_{r+1}, u_{r+2}, \cdots, u_m}_{Null(A^T)}]$$

and for $\mathbb{R}^n$

$$[\underbrace{v_1, v_2, \cdots, v_r}_{Ran(A^T)}, \underbrace{v_{r+1}, v_{r+2}, \cdots, v_n}_{Null(A)}]$$

- Observe $u_i^T A v_j = 0$ for $i > r$ or $j > r$. Therefore

$$U^T A V = R = \begin{pmatrix} C & 0 \\ 0 & 0 \end{pmatrix}_{m\times n} \quad C \in \mathbb{R}^{r\times r} \quad \longrightarrow$$

$$A = URV^T$$

- General class of URV decompositions

- Far from unique.

✍ Show how you can get a decomposition in which C is lower (or upper) triangular, from the above factorization.

- Can select decomposition so that R is upper triangular $\rightarrow$ URV decomposition.
- Can select decomposition so that R is lower triangular $\rightarrow$ ULV decomposition.
- SVD = special case of URV where R = diagonal

✍ How can you get the ULV decomposition by using only the Householder QR factorizatoin (possibly with pivoting)? [Hint: you must use Householder twice]