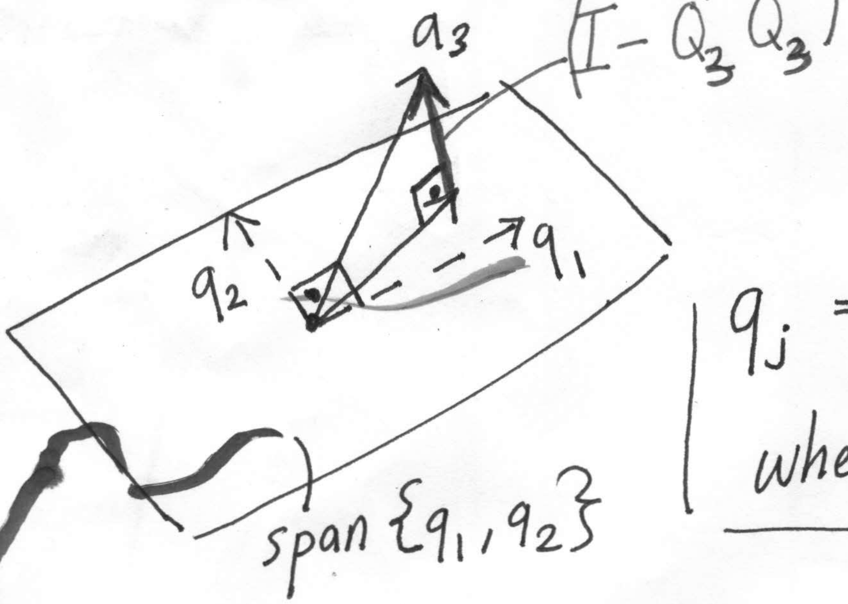
LECTURE 10

MODIFIED GRAM-SCHIMDT

Classical Gram-Schmidt is numerically unstable (i.e. very sensitive to rounding errors).

This is just a reorder of operations so that the Gram-Schmidt procedure becomes numerically stable.



jth iteration of Gram-Schmidt

$$q_j = \frac{(I - \hat{Q}_j \hat{Q}_j^*) a_j}{r_{jj}}$$ scalar to normalize

where $\hat{Q}_j = [q_1 \; q_2 \cdots q_{j-1}]$

$I - \hat{Q}_j \hat{Q}_j^*$: orthogonal projector onto the subspace orthogonal to $S = \text{span}\{q_1, q_2, \dots, q_{j-1}\}$

equivalently

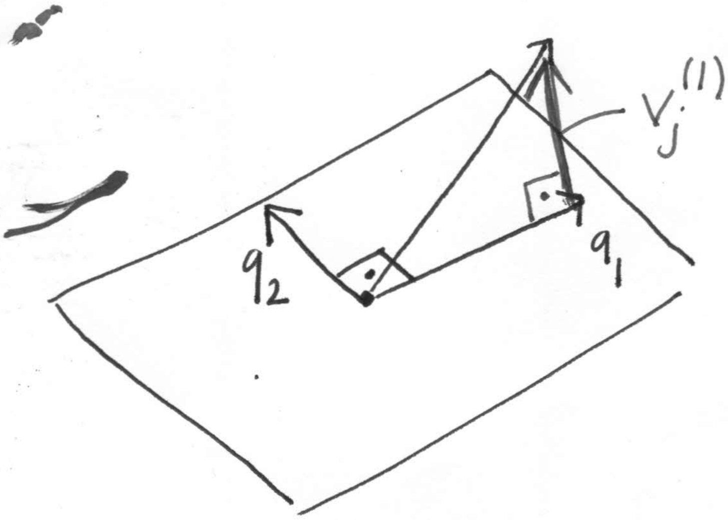
$$q_j = \frac{a_j - (q_1^* a_j) q_1 - \dots (q_{j-1}^* a_j) q_{j-1}}{r_{jj}}$$

Basic Idea:

Instead of projecting onto $S^\perp$ at once (that removes components along $q_1, \dots, q_{j-1}$)

* first project onto the space orthogonal to span$\{q_1\}$ (Remove the component along q_1)

$$v_j^{(1)} = (I - q_1 q_1^*)\, a_j$$

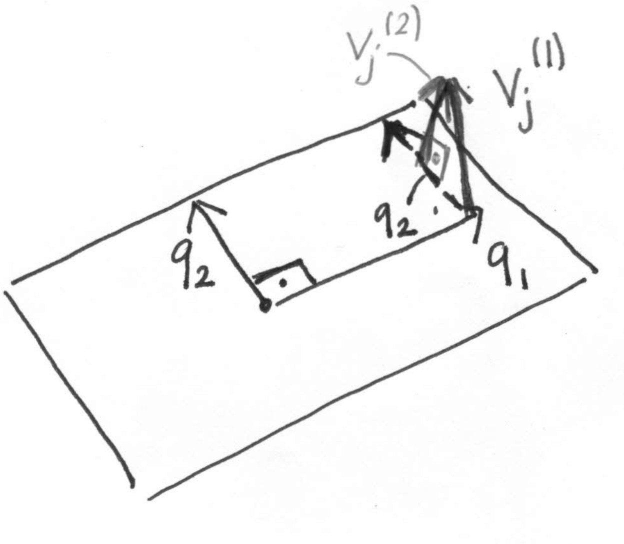


equivalently

$$v_j^{(1)} = a_j - \underbrace{(q_1^* a_j)}_{r_{1j}}\, q_1$$

* then project onto the space orthogonal to span$\{q_2\}$ (Remove the component along q_2)

$$v_j^{(2)} = (I - q_2 q_2^*)\, v_j^{(1)}$$



equivalently

$$v_j^{(2)} = v_j^{(1)} - (q_2^* v_j^{(1)})\, q_2$$

* at the kth iteration (for $k=1,\dots,j-1$) project onto the subspace orthogonal to span $\{q_k\}$ (Remove the component along q_k)

$$v_j^{(k)} = (I - q_k q_k^*)\, v_j^{(k-1)}$$

equivalently

$$v_j^{(k)} = v_j^{(k-1)} - (q_k^* v_j^{(k-1)})\, q_k$$

REMARK

$$v_j^{(j-1)} = (I - q_{j-1} q_{j-1}^*) \dots (I - q_1 q_1^*)\, a_j$$

$$= (I - q_{j-1} q_{j-1}^* - q_{j-2} q_{j-2}^* \dots - q_1 q_1^*)\, a_j$$

(since $\{q_1, q_2, \dots, q_{j-1}\}$ is orthogonal)

$$= (I - \hat{Q}_j \hat{Q}_j^*)\, a_j$$

Therefore define

$$q_j = v_j^{(j-1)} / \| v_j^{(j-1)} \|$$

ALGORITHM (Modified Gram-Schmidt)

* Given $A \in \mathbb{C}^{m \times n}$ (with $m \geq n$)
* Produce $\hat{Q} \in \mathbb{C}^{m \times n}$ (with orthonormal columns) and $\hat{R} \in \mathbb{C}^{n \times n}$ (upper triangular) such that $A = \hat{Q}\hat{R}$.

for $j = 1, \dots, n$ (j : col #)
  $v_j = a_j$
  for $k = 1, \dots, j-1$
    $r_{kj} = q_k^* a_j$
    $v_j = v_j - r_{kj}\, q_k$
  end
  $r_{jj} = \| v_j \|$
  $q_j = v_j / r_{jj}$
end

OPERATION COUNT

The statement $r_{kj} = q_k^* a_j$ requires $2m-1$ flops.

The statement $v_j = v_j - r_{kj}\, q_k$ requires $2m$ flops.

$$\text{Total \# Flops} = \sum_{j=1}^{n}\left(\sum_{k=1}^{j-1} 4m-1\right) + 2m+1$$

$$= \sum_{j=1}^{n} 4m(j-1) + O(m)$$

$$= 4m\,\frac{n(n-1)}{2} + O(mn)$$

$$= \underline{\underline{2mn^2}} + \underbrace{O(mn)}_{cmn}$$

for some constant c

COMPUTING QR-FACTORIZATION BY HOUSEHOLDER REFLECTORS

This is a more efficient way to compute the QR factorization.

(This does not mean that the Gram-Schmidt procedure is useless. The Gram-Schmidt orthogonalization is used to calculate a partial QR factorization inside the Krylov-based methods for linear systems and eigenvalues.)

Overview of the algorithm (on a 3×3 matrix)

$$A = \begin{bmatrix} \boxed{\begin{matrix} x \\ x \\ x \end{matrix}} & \begin{matrix} x \\ x \\ x \end{matrix} & \begin{matrix} x \\ x \\ x \end{matrix} \end{bmatrix} \xrightarrow{\quad Q_1 \quad} \begin{bmatrix} x & x & x \\ 0 & \boxed{\begin{matrix} x \\ x \end{matrix}} & \begin{matrix} x \\ x \end{matrix} \end{bmatrix} \xrightarrow{\quad Q_2 \quad} \begin{bmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \end{bmatrix} = R$$

Define the Householder reflector Q_1 in terms of this vector

define HH reflector Q_2 in terms of this

Householder reflectors will be applied from the left.

$$Q_2 Q_1 A = R \Longrightarrow \underbrace{Q_1^* Q_2^* Q_2 Q_1}_{I} A = Q_1^* Q_2^* R$$

$$\Longrightarrow A = \underbrace{Q_1^* Q_2^*}_{Q \text{ (unitary)}} R$$

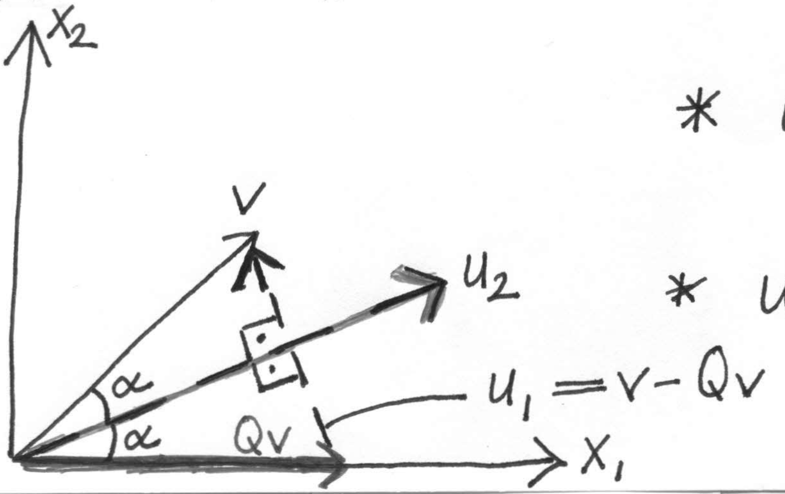
Householder Reflector

A unitary matrix $Q \in \mathbb{C}^{m \times m}$ that satisfies (for a given vector $v \in \mathbb{C}^m$)

$$v \longrightarrow Qv = \begin{bmatrix} \|v\| \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \|v\| e_1$$

(Recall that the vector 2-norm is preserved under unitary transformations. Therefore $\|v\| = \|Qv\|$)

Suppose $v \in \mathbb{R}^2$



$*$ $u_1 = \dfrac{v - Qv}{\|v - Qv\|}$

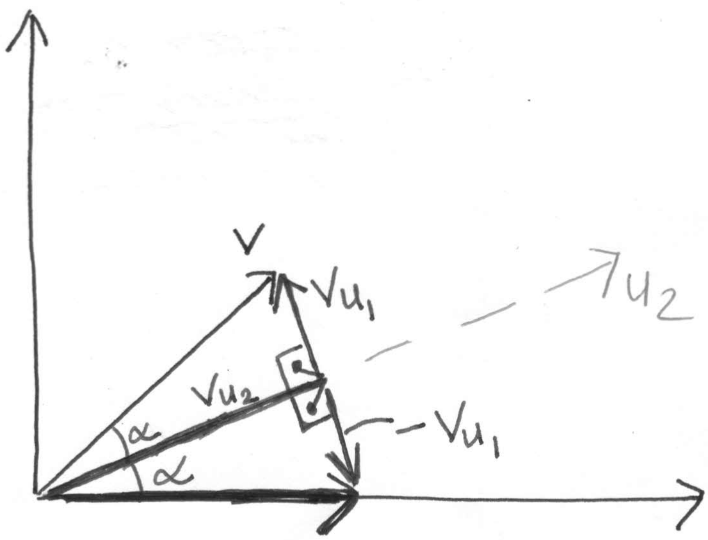
$*$ $u_2 \perp u_1$ and $\|u_2\| = 1$

Q is the transformation that reflects v about u_2.

$$v = v_{u_1} + v_{u_2}$$

v_{u_1} : orthogonal projection of v onto u_1

v_{u_2} : orthogonal projection of v onto u_2



$$Qv = \|v\| e_1$$

$$\begin{aligned} Qv &= -v_{u_1} + v_{u_2} \\ &= -v_{u_1} + (v - v_{u_1}) \\ &= v - 2v_{u_1} \\ &= v - 2\left((u_1 u_1^T) v\right) \\ &= \left(I - 2u_1 u_1^T\right) v \end{aligned}$$

$Q = I - 2u_1u_1^T$ is called the Householder reflector.

REMARK

$Q = I - 2u_1u_1^T$ is an orthogonal matrix.

$$\begin{aligned} Q^TQ &= (I - 2u_1u_1^T)^T (I - 2u_1u_1^T) \\ &= (I - 2u_1u_1^T)(I - 2u_1u_1^T) \\ &= I - 4u_1u_1^T + 4(u_1 \underbrace{u_1^Tu_1}_{1} u_1^T) \\ &= I \end{aligned}$$

EXAMPLE

Find the QR factorization for

$$A = \begin{bmatrix} 3 & 1 \\ 4 & 2 \end{bmatrix}$$

Determine the Householder reflector Q such that

$$v = \begin{bmatrix} 3 \\ 4 \end{bmatrix} \longrightarrow Qv = \begin{bmatrix} \|v\| \\ 0 \end{bmatrix} = \begin{bmatrix} 5 \\ 0 \end{bmatrix}$$

(1) Find u_1

$$u_1 = \frac{(v - Qv)}{\|v - Qv\|}$$

$$= \frac{(v - \|v\|e_1)}{\|v - \|v\|e_1\|} = \frac{1}{\sqrt{20}}\begin{bmatrix} -2 \\ 4 \end{bmatrix}$$

(2) Find the Householder reflector reflecting about u_2 where $u_2 \perp u_1$ and $\|u_2\|_2 = 1$

$$Q = I - 2u_1 u_1^T$$

$$= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - 2\left(\frac{1}{\sqrt{20}}\begin{bmatrix} -2 \\ 4 \end{bmatrix}\right)\left(\frac{1}{\sqrt{20}}\begin{bmatrix} -2 & 4 \end{bmatrix}\right)$$

$$= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \frac{1}{10}\begin{bmatrix} 4 & -8 \\ -8 & 16 \end{bmatrix}$$

$$= \begin{bmatrix} 0.6 & 0.8 \\ 0.8 & -0.6 \end{bmatrix} \quad \left(\begin{array}{c}\text{Note that} \\ Q^TQ = I\end{array}\right)$$

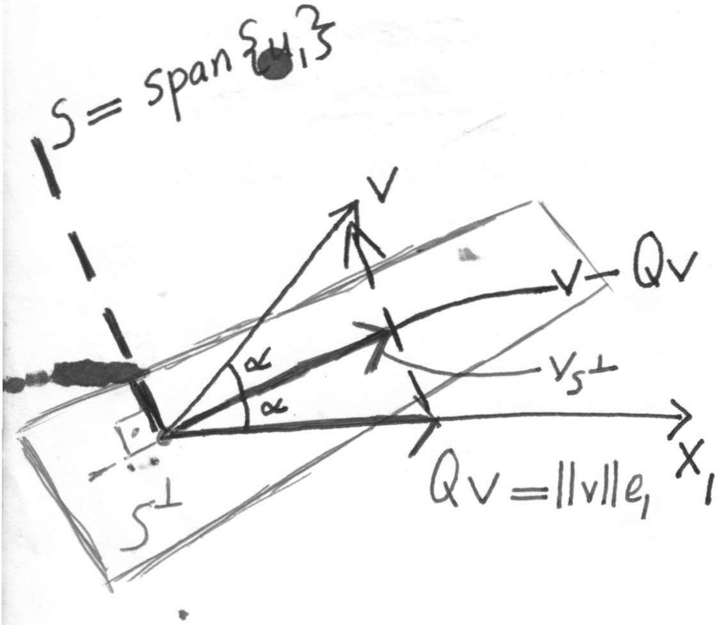
(3) Determine the QR factorization

$$QA = \begin{bmatrix} 0.6 & 0.8 \\ 0.8 & -0.6 \end{bmatrix}\begin{bmatrix} 3 & 1 \\ 4 & 2 \end{bmatrix} = \underbrace{\begin{bmatrix} 5 & 2.2 \\ 0 & -0.4 \end{bmatrix}}_{R}$$

$$\Longrightarrow A = Q^T R$$
$$= QR$$
$$= \begin{bmatrix} 0.6 & 0.8 \\ 0.8 & -0.6 \end{bmatrix} \begin{bmatrix} 5 & 2.2 \\ 0 & -0.4 \end{bmatrix}$$

Suppose $v \in \mathbb{C}^m$. Householder reflector $Q \in \mathbb{C}^{m \times m}$ must satisfy

$$v \longrightarrow Qv = \|v\| e_1$$



$* \; u_1 = \dfrac{v - Qv}{\|v - Qv\|}$

$* \; S^\perp$ is the subspace orthogonal to u_1

Q is the transformation that reflects about $S^\perp$.

$$v = v_S + v_{S^\perp}$$

$$\boxed{Q - \text{Householder reflector} \quad Q = I - 2u_1u_1^*}$$

$$\begin{aligned} Qv &= -v_S + v_{S^\perp} \\ &= -v_S + (v - v_S) \\ &= v - 2v_S \\ &= v - 2\big((u_1u_1^*)v\big) = (I - 2u_1u_1^*)v \end{aligned}$$