

- How to compute QR factorization?

Idea 1: convert basis to orthonormal one

Gram-Schmidt: given  $a_1, \dots, a_n \in \mathbb{C}^m$ , produce orthonormal  $q_1, \dots, q_n$  with  $\text{span}\{q_1, \dots, q_n\} = \text{span}\{a_1, \dots, a_n\}$

$$\begin{aligned} q_1 &= \frac{a_1}{\|a_1\|_2} \\ q'_2 &= a_2 - (q_1^* a_2) q_1, \quad q_2 = \frac{q'_2}{\|q'_2\|_2} \\ &\dots \\ q'_j &= a_j - \sum_{i=1}^{j-1} (q_i^* a_j) q_i, \quad q_j = \frac{q'_j}{\|q'_j\|_2} \quad j=3, \dots, n \end{aligned}$$

$$\Leftrightarrow \begin{aligned} a_1 &= \|a_1\|_2 q_1 \\ a_2 &= (q_1^* a_2) q_1 + q_2 \|a_2 - (q_1^* a_2) q_1\|_2 \\ &\dots \\ a_j &= \sum_{i=1}^{j-1} (q_i^* a_j) q_i + q_j \|a_j - \sum_{i=1}^{j-1} (q_i^* a_j) q_i\|_2 \end{aligned}$$

$$\Leftrightarrow \begin{aligned} A &= QR \\ A = [a_1 \dots a_n], \quad R_{ij} &= \begin{cases} q_i^* a_j, & i < j \\ \|a_j - \sum_{k=1}^{j-1} (q_k^* a_j) q_k\|_2, & i = j \\ 0, & \text{otherwise} \end{cases} \end{aligned}$$

Implementation:

Classical GS Input:  $A \in \mathbb{C}^{m \times n}$  of rank  $n$

Output:  $Q \in \mathbb{C}^{m \times n}$ ,  $R \in \mathbb{C}^{n \times n}$

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for j = 1, ..., n
  for i = 1, ..., j-1          * operation count:
     $R_{ij} = q_i^* a_j \rightarrow (j-1)(2m-1)$ 
  end
   $q'_j = a_j - \sum_{i=1}^{j-1} R_{ij} q_i \rightarrow 2m(j-1)$ 
   $R_{jj} = \|q'_j\|_2$ 
   $q_j = q'_j / R_{jj}$ 
end
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$\sum_{j=1}^n (j-1)(2m-1) + 2(j-1)m + 2m + m$

$\approx \sum_{j=1}^n 4jm$

$\approx 2mn^2 \text{ FLOPs}$

- weakness: there is nothing to force orthogonality of  $Q$  in classical Gram-Schmidt

ex.  $A = \begin{bmatrix} 1 & 1 & 1 \\ \varepsilon & & \\ & \varepsilon & \\ & & \varepsilon \end{bmatrix}$

assume  $\varepsilon$  so small such that  $1/(1+\varepsilon^2) \approx 1$

then  $Q_{GS} = \begin{bmatrix} 1 & 0 & 0 \\ \varepsilon & -1/\sqrt{2} & -1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 0 \\ 0 & 0 & 1/\sqrt{2} \end{bmatrix}$

$q_1 \quad q_2 \quad q_3$

$$q_2^* q_3 = \frac{1}{2}$$

- Remedy: Instead of orthogonalizing  $a_j$  at step  $j$  only, can orthogonalize  $a_j$  to  $q_i$  as soon as  $q_i$  is computed

## modified GS

Let  $a_k^{(1)} = a_k$ ,  $k = 1, \dots, n$

for  $k = 1, \dots, n$

operation counts  
 $\approx 2mn^2$

$$R_{kk} = \|a_k^{(k)}\|_2, \quad q_k = a_k^{(k)} / R_{kk}$$

for  $j = k+1, \dots, n$

$$R_{kj} = q_k^* a_j^{(k)}, \quad a_j^{(k+1)} = a_j^{(k)} - R_{kj} q_k$$

end

end

classical GS is equivalent to modified GS  $\leftarrow$  exercise

Thm Suppose Modified GS is applied to  $A \in \mathbb{R}^{m \times n}$  of rank  $n$  yielding  $\hat{Q} \in \mathbb{R}^{m \times n}$ ,  $\hat{R} \in \mathbb{R}^{n \times n}$ ,

$\exists C_i = C_i(m, n)$ , s.t.

$$A + \Delta A_1 = \hat{Q} \hat{R}, \quad \|\Delta A_1\|_2 \leq C_1 \epsilon_{\text{mach}} \|A\|_2$$

$$\|\hat{Q}^T \hat{Q} - I\|_2 \leq C_2 \epsilon_{\text{mach}} K_2(A) / (1 - C'_2 \epsilon_{\text{mach}} K_2(A))$$

and  $\exists Q \in \mathbb{R}^{m \times n}$  with orthonormal columns s.t.

$$\hat{R} \text{ is the exact triangular QR factor of a matrix near Pf: } A + \Delta A_2 = Q \hat{R}, \quad \|\Delta A_2\|_2 \leq C_3 \epsilon_{\text{mach}} \|A\|_2$$

$$\|Q - \hat{Q}\|_2 \leq C_4 \epsilon_{\text{mach}} K_2(A) / (1 - C'_4 \epsilon_{\text{mach}} K_2(A))$$

$\hat{R}$  is the exact triangular QR factor of a matrix near Pf: to A.

i.e. it is a good R-factor.

Higham Thm 9.13  $\square$

The departure from orthonormality of  $\hat{Q}$  is bounded by  $O(K_2(A) \epsilon_{\text{mach}})$

- Back to least-squares:

Solve least-squares via QR:  $\|b + \Delta b - (A + \Delta A)y\|_2^2$

$$\hat{x} = \hat{R}^{-1} \hat{Q}^* b$$

use  $\hat{Q}^* \hat{Q} = I_n$  suffer from large  $K_2(A)$

Instead, we can apply Modified GS to  $[A \ b]$

$$[A \ b] = [Q_1 \ q_{n+1}] \begin{bmatrix} R & z \\ 0 & p \end{bmatrix}$$

$$\text{We have } Ax - b = [A \ b] \begin{bmatrix} x \\ -1 \end{bmatrix}$$

$$= [Q_1 \ q_{n+1}] \begin{bmatrix} Rx - z \\ -p \end{bmatrix}$$

$$= Q_1 (Rx - z) - p q_{n+1}$$

$$\text{Hence } \|Ax - b\|_2^2 = \|Rx - z\|_2^2 + p^2$$

So  $x = R^{-1}z$  is the Least-squares solution

Thm Solving LS via Modified GS for  $[A \ b]$

has forward error as good as a backward stable algo.

- Can perform QR factorization faster than  $2mn^2$  FLOPs if don't need to form  $Q$  explicitly

\* Householder:

$$A \begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \\ x & x & x \end{pmatrix} \xrightarrow{Q_1} \begin{pmatrix} x & x & x \\ 0 & x & x \\ 0 & x & x \\ 0 & x & x \end{pmatrix} \xrightarrow{Q_2} \begin{pmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \\ 0 & 0 & x \end{pmatrix} \xrightarrow{Q_3} \begin{pmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \\ 0 & 0 & 0 \end{pmatrix}$$

$\begin{bmatrix} 1 & 0 \\ 0 & H_2 \end{bmatrix}$ 
 $\begin{bmatrix} 1 & 0 \\ 0 & H_3 \end{bmatrix}$

$$Q_3 Q_2 Q_1, A = \begin{bmatrix} R \\ 0 \end{bmatrix} \Rightarrow A = (Q_3 Q_2 Q_1)^* \begin{bmatrix} R \\ 0 \end{bmatrix}$$

$Q_i$  unitary

$$= Q \begin{bmatrix} R \\ 0 \end{bmatrix} \leftarrow \text{full QR}$$

$Q \in \mathbb{C}^{m \times n}$  unitary

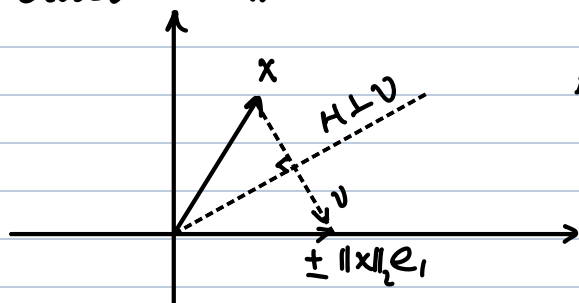
\* How to choose  $Q_k$ ?

$\begin{bmatrix} R \\ 0 \end{bmatrix} \in \mathbb{C}^{m \times n}$  upper triangular

$$\text{Let } Q_k = \begin{bmatrix} I_{k-1} & 0 \\ 0 & H_k \end{bmatrix} \begin{matrix} k-1 \\ m-(k-1) \end{matrix}, \quad H_k \text{ unitary (thus norm preserving)}$$

$x \in \mathbb{C}^{m-(k-1)}$  be  $k$ th, ...,  $m$ th entries of  $k$ th column

Goal:  $H_k x = \pm \|x\|_2 e_1$



Householder transform:  
reflection across the plane  $H$

$$\begin{aligned} H_k x &= x - 2 P_v x = x - 2 \left( \frac{v^*}{\|v\|_2} x \right) \frac{v}{\|v\|_2} \\ &= \underbrace{\left( I - \frac{2 v v^*}{\|v\|_2^2} \right)}_{\text{Householder transform}} x \end{aligned}$$

(a) For stability, one may choose  $v = \text{sign}(x_1) \|x\|_2 e_1 + x$  to avoid catastrophic cancellation in computing  $\|v\|_2^2$  when  $\|x\| \approx |x_1|$    
  $\uparrow$  why?

(b) Householder matrices  $H_k$  is never formed in upper triangularizing  $A$ , storage and computations use solely the Householder vector  $v$ .

- Implementation:

Householder QR:

For  $k = 1, \dots, n$

$$x \leftarrow A(k:m, k)$$

$$v_k = \text{sign}(x_1) \|x\|_2 e_1 + x$$

$$v_k \leftarrow v_k / \|v_k\|_2$$

$$A(k:m, k:n) \leftarrow A(k:m, k:n) - 2 v_k (v_k^* A(k:m, k:n))$$

end

- operation count:

$$\approx \sum_{k=1}^n 4(m-k)(n-k) \text{ FLOPs}$$

$$\approx 4 \left( mn^2 - (m+n) \frac{n^2}{2} + \frac{n^3}{3} \right)$$

$$\approx 2mn^2 - \frac{2}{3}n^3$$

subtraction  
(m-k)(n-k)  
FLOPs

outer product  
(m-k)(n-k)  
FLOPs

matrix-vector product  
2(m-k)(n-k) FLOPs

- Stability of Householder transform

Since the orthogonal transform is performed by Householder vector, the orthogonality of  $Q$  is enforced

Thm Let  $\begin{bmatrix} \hat{R} \\ 0 \end{bmatrix} \in \mathbb{R}^{m \times n}$  be the computed upper triangular QR

factor of  $A \in \mathbb{R}^{m \times n}$ , Let  $Q = (\hat{Q}_n \dots \hat{Q}_1)^T$  be

the exact orthogonal matrix obtained from Householder

vectors computed from the algorithm

Then  $A + \Delta A = Q \hat{R}$  with  $\|\Delta A\|_2 \leq C_{m,n} \|A\|_2$

Let  $\hat{Q} = \text{fl}((\hat{Q}_n \dots \hat{Q}_1)^T)$  be the computed orthogonal matrix

Then  $\hat{Q} = Q(I_m + \Delta I)$  with  $\|\Delta I\|_2 \leq C_{m,n}$



$\hat{Q}$  is very close to orthogonal matrix  
regardless of  $K(A)$ !

This a consequence of the backward stability of  
matrix multiplication

- Back to solve least-squares

Solve least-squares via QR:

$$\hat{x} = \hat{R}^{-1} \hat{Q}^* b$$

use  $\hat{Q}^* \hat{Q} = I_n$  NOT suffer from large  $K_2(A)$

Thm Let  $A \in \mathbb{R}^{m \times n}$  have full rank and that the least square problem  $\min_x \|Ax - b\|_2$  is solved using Householder QR factorization. The computed solution  $\hat{x}$  is the exact solution to

$$\min_x \|b + \Delta b - (A + \Delta A) \hat{x}\|_2$$

$$\text{where } \|\Delta A\|_2 \leq C_{\min} \|A\|_2, \quad \|\Delta b\|_2 \leq C_{\min} \|b\|_2$$

↑  
Backward stable!

Summary:

operation count:  
 $O(2mn^2)$

$O(4mn^2)$

normal equation < Householder QR < Modified GS < SVD  
(without computing  $Q$  explicitly) (Augmented)

Rounding error:

$O(K_2^2(A) \epsilon_{\text{mach}})$

$O(K_2(A) \epsilon_{\text{mach}})$

normal equation > Householder QR  $\approx$  Modified GS  $\approx$  SVD  
(without computing  $Q$  explicitly) (Augmented)