- How to compute QR factorization?

Idea 1: convert basis to orthonormal one

Gram – Schmidt: given $a_1, \cdots, a_n \in \mathbb{C}^m$, produce orthonormal $q_1, \cdots, q_n$ with $\operatorname{span}\{q_1, \cdots, q_n\} = \operatorname{span}\{a_1, \cdots, a_n\}$

$$q_1 = \frac{a_1}{\|a_1\|_2}$$

$$q_2' = a_2 - (q_1^* a_2) q_1, \qquad q_2 = \frac{q_2'}{\|q_2'\|_2}$$

$$\cdots$$

$$q_j' = a_j - \sum_{i=1}^{j-1} (q_i^* a_i) q_i, \qquad q_j = \frac{q_j'}{\|q_j'\|_2} \qquad j = 3, \cdots, n$$

$\Longleftrightarrow$

$$a_1 = \|a_1\|_2 q_1$$

$$a_2 = (q_1^* a_2) q_1 + q_2 \| a_2 - (q_1^* a_2) q_1 \|_2$$

$$\cdots$$

$$a_j = \sum_{i=1}^{j-1} (q_i^* a_i) q_i + q_j \| a_j - \sum_{i=1}^{j-1} (q_i^* a_i) q_i \|_2$$

$\Longleftrightarrow$

$$A = QR$$

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

Implementation :

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

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

for $j = 1, \cdots, n$

for $i = 1, \cdots, j-1$ $\quad$ * operation count:

$R_{ij} = q_i^* a_j \longrightarrow (j-1)(2m-1)$ $\quad$ $\sum_{j=1}^{n} (j-1)(2m-1) + 2(j-1)m + 2m + m$

end

$q_j' = a_j - \sum_{i=1}^{j-1} R_{ij}\, q_i \longrightarrow 2m(j-1)$ $\quad$ $\approx \sum_{j=1}^{n} 4jm$

$R_{jj} = \|q_j'\|_2 \longrightarrow 2m$, $\quad q_j = q_j' / R_{jj} \longrightarrow m$ $\quad$ $\approx 2mn^2$ FLOPs

end

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

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

assume ε so small such that $fl(1+\varepsilon^2) = 1$

then $Q_{GS} = \begin{array}{c} \begin{bmatrix} 1 & 0 & 0 \\ \varepsilon & -1/\sqrt{2} & -1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 0 \\ 0 & 0 & 1/\sqrt{2} \end{bmatrix} \\ \begin{matrix} q_1 & \quad q_2 & \quad q_3 \end{matrix} \end{array}$

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

- 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 $a_k^{(1)} = a_k$, $k = 1, \cdots, n$

operation counts $\approx 2mn^2$

for $k = 1, \cdots, n$

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

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

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

end

end

classical GS is equivalent to modified GS ← 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.

$$A + \Delta A_1 = \hat{Q}\hat{R}, \quad \|\Delta A_1\|_2 \le c_1 \varepsilon_{mach} \|A\|_2$$

$$\|\hat{Q}^T \hat{Q} - I\|_2 \le c_2 \varepsilon_{mach} \kappa_2(A) / (1 - c_2' \varepsilon_{mach} \kappa_2(A))$$

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

$\hat{R}$ is the exact triangular QR factor of a matrix near to A. i.e. it is a good R-factor. →

$$A + \Delta A_2 = Q\hat{R}, \quad \|\Delta A_2\|_2 \le c_3 \varepsilon_{mach} \|A\|_2$$

$$\|Q - \hat{Q}\|_2 \le c_4 \varepsilon_{mach} \kappa_2(A) / (1 - c_4' \varepsilon_{mach} \kappa_2(A))$$

Pf: Higham Thm 19.13 ∎

The departure from orthonormality of $\hat{Q}$ is bounded by $O(\kappa_2(A)\, \varepsilon_{mach})$

- Back to least-squares :

If we translation the result to backward error analysis, we get that the computed $\hat{x}$ is the exact solution of the LS problem $\| b+\Delta b - (A+\Delta A) y \|_2^2$

Solve least-squares via QR :

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

where $\|\Delta b\|_2 / \|b\|_2 \lesssim \kappa_2(A)\,\varepsilon_{mach}$, $\|\Delta A\|_2/\|A\|_2 \lesssim \varepsilon_{mach}$

NOT Backward stable

use $\hat{Q}^*\hat{Q} = I_n$ suffer from large $\kappa_2(A)$

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

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

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

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

$$= Q_1 (Rx - z) - \rho\, q_{n+1}$$

Hence $\quad \|Ax-b\|_2^2 = \|Rx - z\|_2^2 + \rho^2$

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

<u>Thm</u> 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 :

$$\overset{A}{\begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \\ x & x & x \end{pmatrix}} \xrightarrow{Q_1} \begin{pmatrix} x & x & x \\ 0 & x & x \\ 0 & x & x \\ 0 & x & x \end{pmatrix} \xrightarrow{Q_2 = \begin{bmatrix} 1 & 0 \\ 0 & H_2 \end{bmatrix}} \begin{pmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \\ 0 & 0 & x \end{pmatrix} \xrightarrow{Q_3 = \begin{bmatrix} 1 & \\ & 1 & \\ & & H_3 \end{bmatrix}} \begin{pmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \\ 0 & 0 & 0 \end{pmatrix}$$

H_2

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

Q_i unitary

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

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

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

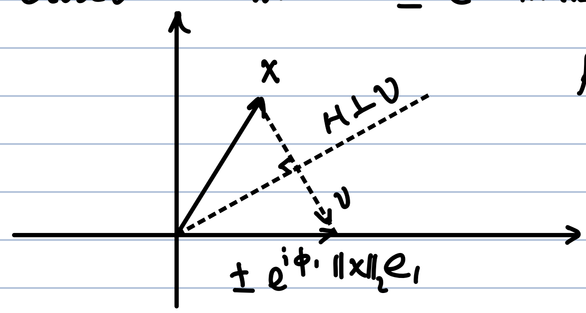
* How to choose Q_k?

Let
$$Q_k = \begin{array}{cc} \begin{array}{cc} k-1 & m-(k-1) \end{array} & \\ \begin{bmatrix} I & 0 \\ 0 & H_k \end{bmatrix} & \begin{array}{c} k-1 \\ m-(k-1) \end{array} \end{array},$$
H_k unitary (thus norm preserving)

keep the first $k-1$ coordinates unchanged

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

Goal: $H_k x = \pm e^{i\phi_1} \|x\|_2 e_1$ $\quad \begin{pmatrix} \times \\ \times \\ \times \end{pmatrix} \xrightarrow{H_k} \begin{pmatrix} \times \\ 0 \\ 0 \end{pmatrix}$



Householder transform: reflection across the plane H

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

$\phi_1 = \arg(x_1)$ is added to make $x, \pm e^{i\phi_1}\|x\|_2 e_1$ symmetric with respect to H, i.e. $v^* x = -v^*(\pm e^{i\phi_1}\|x\|_2 e_1)$. Such that $H_k x = \pm e^{i\phi_1}\|x\|_2 e_1$ (otherwise H_k doesn't reflect x to $\pm e^{i\phi_1}\|x\|_2 e_1$!)

(a) For stability, one may choose $v = e^{i\phi_1}\|x\| e_1 + x$ to avoid catastrophic cancellation in computing $\|v\|_2^2$ when $\|x\|_2 \approx |x_1|$ ← 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 $k = 1, \cdots, n$

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

$v_k = \text{sign}(x(1)) \|x\|_2 e_1 + x$

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

substraction $(m-k)(n-k)$ FLOPs

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

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

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

end

- operation count:

$$\approx \sum_{k=1}^{n} 4(m-k)(n-k) \quad \text{FLOPs}$$
$$\approx 4\left(mn^2 - (m+n)\frac{n^2}{2} + \frac{n^3}{3}\right)$$
$$\approx 2mn^2 - \frac{2}{3}n^3$$

- Stability of Householder transform

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

<u>Thm</u> 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 $Q = (\hat{Q}_n \cdots \hat{Q}_1)^T$ be the exact orthogonal matrix obtained from Householder vectors computed from the algorithm

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

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

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

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

This a consequence of the backward stability of matrix multiplication

- Back to solve least-squares

Solve least-squares via QR:

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

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

<u>thm</u> 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

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

where $\|\Delta A\|_2 \le C_{mn} \|A\|_2$, $\|\Delta b\|_2 \le C_{mn} \|b\|_2$

Backward stable!

Summary:

Operation count:

$O(2mn^2)$ | $O(4mn^2)$

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

Rounding error:

$O(K_2^2(A)\,\varepsilon_{mach})$ | $O(K_2(A)\,\varepsilon_{mach})$

normal equation > Householder QR (without computing Q explicitly) ≈ Modified GS (Augmented) ≈ SVD