Welcome to Ma 221! Lecture 18, Oct 4

Algorithms for $A^{m\times n} = QR$

Classical + Modified Gram-Schmidt

CGS + MGS

Equate columns of A and QR

$$A(:,i) = \sum_{j=1}^{i} Q(:,j)\cdot R(j,i)$$

since columns of Q orthogonal

$$(Q(:,j))^T A(:,i) = R(j,i)$$

for $i = 1:n$

  $tmp = A(:,i)$

  for $j = 1:i-1$

2m flops $R(j,i) = (Q(:,j))^T \cdot A(:,i)$ ... CGS

" $R(j,i) = (Q(:,j))^T \cdot tmp$ ... MGS

" $tmp = tmp - R(j,i)\cdot Q(:,j)$

  end for ... $tmp = R(i,i)\cdot Q(:,i)$

" $R(i,i) = \|tmp\|_2$

m flops $Q(:,i) = tmp / R(i,i)$

end for

$\#$ flops $= 2mn^2 + O(mn)$

$\sim 2\times$ cost of NE if $m \gg n$

Householder - stable
MGS - less stable
CGS - even less stable) still used, because Q returned explicitly
but for Householder Q implicit

2 Metrics of Backward Stability

want accurate decomposition $A = QR$

$$A + E = QR \quad , \quad \|E\| = O(\varepsilon)\cdot\|A\|$$

$$\frac{\|A - QR\|}{\|A\|} = O(\varepsilon)$$

want Q to be close to orthogonal

$$\|Q^T Q - I\| = O(\varepsilon)$$

How to "fix" CGS and MGS: do them twice
i.e. run it again on output Q, better, not perfect

Perturbation Theory for LS

How much can $x = \operatorname{argmin}_x \|Ax - b\|_2$ change if A and b change?

When $m = n$, same as solving $Ax = b$
so expect $\kappa(A) = \frac{\sigma_{max}}{\sigma_{min}}$ to appear

Another source of ill-conditioning

$$A = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \; b = \begin{bmatrix} 0 \\ b_2 \end{bmatrix} \qquad x = [1, 0]\cdot\begin{bmatrix} 0 \\ b_2 \end{bmatrix} = 0$$

$$A = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \; b = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \qquad x = [1, 0]\cdot\begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = b_1$$

$\Rightarrow$ large relative change in x

In general, ill conditioned if b (nearly) orthogonal to span(A)

$$x+e = \arg\min_x \|(A+\delta A)x - (b+\delta b)\|_2$$

$$x = \arg\min_x \|Ax - b\|_2$$

$$e = (x+e)-x = ((A+\delta A)^T(A+\delta A))^{-1}(A+\delta A)^T(b+\delta b) - (A^TA)^{-1}A^Tb$$

Do Taylor expansion, keep first term

$$(I-X)^{-1} = I + X + O(X^2)$$

ignore

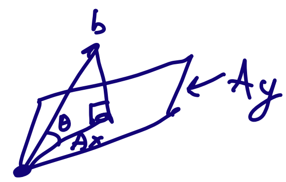
only keep terms with one "small" factor δA or δb

Def: $\varepsilon = \max\left(\dfrac{\|\delta A\|_2}{\|A\|_2}, \dfrac{\|\delta b\|_2}{\|b\|_2}\right)$

$$\frac{\|e\|_2}{\|x\|_2} \le \varepsilon\left(2\cdot K(A)\cdot\frac{1}{\cos\theta} + \tan\theta\cdot K^2(A)\right) + O(\varepsilon^2)$$

$\theta =$ angle(b, Ax)

$\sin(\theta) = \dfrac{\|Ax-b\|_2}{\|b\|_2}$



$\theta = 0 \Rightarrow \dfrac{\|e\|}{\|x\|} \le \varepsilon(2\cdot K(A))$ ... best case

condition number large when:

1. $K(A)$ large
2. θ near $\frac{\pi}{2} \Rightarrow \frac{1}{\cos\theta}, \tan\theta$ large
3. error like $K^2(A)$ when θ not near 0

Householder: Stable Alg for QR

Represent Q as product $Q = Q_1 \cdot Q_2 \cdots Q_n$ of "simple" orthogonal Q_i, chosen to make progress zeroing out entries of A to turn it into R

2 kinds of "simple" Q_i:

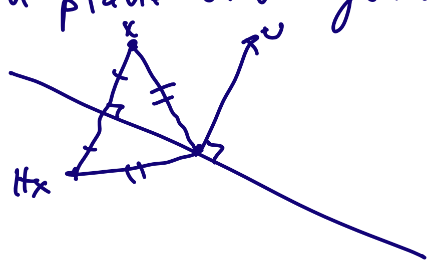
Householder Transformation (reflections)

Givens rotations $\begin{bmatrix} c & s \\ -s & c \end{bmatrix}$ $\quad c = \cos\theta$, $s = \sin\theta$

Householder: $H = I - 2uu^T$, $\|u\|_2 = 1$

$$HH^T = (I - 2uu^T)(I - 2uu^T)$$
$$= I - 2uu^T - 2uu^T + 4u\underbrace{u^Tu}_{=1}u^T = I$$

Reflection Hx is reflection of x in plane orthogonal to u



Given x, choose u so Hx has zeros in certain locations

$$Hx = \begin{bmatrix} c \\ 0 \\ \vdots \\ 0 \end{bmatrix} = c \cdot e_1 \text{ for some } c$$

$$\|Hx\|_2 = \|x\|_2 = |c| \Rightarrow c = \pm\|x\|_2$$

$$Hx = (I - 2uu^T)x = x - 2u\underbrace{u^Tx} = c \cdot e_1$$

$$\Rightarrow u = \frac{x - ce_1}{2u^Tx}$$

denominator scalar, choose it so $\|u\|_2 = 1$

$$y = x - ce_1 = x \pm \|x\|_2 \cdot e_1$$

$$u = \frac{y}{\|y\|_2}$$

$$u = \text{House}(x)$$

How to pick sign of $\pm\|x\|_2$: choose to avoid cancellation in

$$y = \begin{bmatrix} x_1 \pm \|x\|_2 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} x_1 + \text{sign}(x_1)\cdot\|x\|_2 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

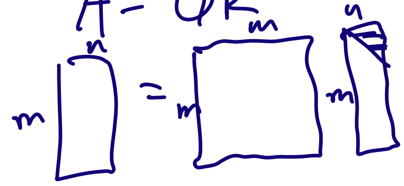
(may get R_{ii} positive or negative)

$$\underbrace{\begin{bmatrix} I^3 & 0 \\ 0 & H^{2\times2} \end{bmatrix} \begin{bmatrix} \begin{smallmatrix}1&0\\0&1\end{smallmatrix} & 0 \\ 0 & H^{3\times3} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & H^{4\times4} \end{bmatrix} H^{5\times5}}_{Q^T} \cdot \underset{A^{5\times4}}{\begin{bmatrix} x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \end{bmatrix}} = R$$

product of 4 orthogonal matrices, so $= Q^T$

Q implicit

$$A = QR$$



$$\text{need } (I - 2uu^T)A = A - 2u\underbrace{(u^TA)}_{\substack{\text{mat vec}\\ \text{GEMV}}}$$

GER rank 1 update

QR for $A^{m \times n}$ $\quad m \geq n$

for $i = 1$ to $\min(m-1, n)$ .. only need to do last col if $m > n$

$u(i) = \text{House}(A(i:m, i))$

$A(i:m, i:n) = (I - 2u(i)u(i)^T)\, A(i:m, i:n)$

$= A(i:m, i:n) - 2u(i) \cdot \underbrace{(\underbrace{(u(i))^T A(i:m, i:n)}_{\text{GEMV}})}_{\text{GER}}$

Where store $u(i)$s? same trick as storing L in GE: in zero entries below diagonal of A

$$\text{Cost} = \sum_{i=1}^{n} 4(m-i+1)(n-i+1) = 2n^2 m - \frac{2}{3} n^3$$

$m \gg n$: dominated by $2n^2 m$

$m = n$: $\frac{4}{3} n^3$, twice GE

Solve LS using implicit Q.

$Q_n \cdots Q_2 Q_1 A = R$

$A = Q_1^T Q_2^T \cdots Q_n^T R$

$x = R^{-1} Q^T b = \underset{x}{\operatorname{argmin}} \|Ax - b\|_2$

for $i = 1$ to n

$b = Q_i b = (I - 2u_i u_i^T) b$

$= \underbrace{b - 2u_i \underbrace{(u_i^T b)}_{\text{dot product}}}_{\text{axpy}}$

endfor

$b = R^{-1} b$

$\Longrightarrow$ cost $= O(m \cdot n)$ much less than QR