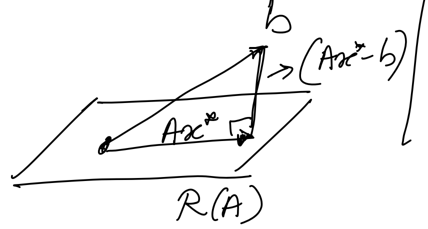
The Least Squares Problem : $A \in \mathbb{R}^{m\times n}, b \in \mathbb{R}^m$

$$\min_{x\in\mathbb{R}^n} \|Ax - b\|_2$$



$$\underset{m\times n}{\begin{bmatrix} \\ A \\ \\ \end{bmatrix}} \underset{n\times 1}{\begin{bmatrix} x \end{bmatrix}} \approx \underset{m\times 1}{\begin{bmatrix} \\ b \\ \\ \end{bmatrix}}$$

Normal Eqns :

FACT: x solves the L.S. problem iff

$$A^TAx = A^Tb \longrightarrow \text{normal eqns}$$

FACT: a) Normal eqns are always consistent

b) When A is full rank, the unique solution is given by $\hat{x} = (A^TA)^{-1}A^Tb$

c) When A is not full rank, the normal eqn always have more than one solution, where any two solutions $\hat{x}_1$ & $\hat{x}_2$ satisfy $A(\hat{x}_1 - \hat{x}_2) = 0$

d) The projection of b onto $R(A)$ is unique & is defined by $\hat{b} := A\hat{x}$, where $\hat{x}$ is any solution to the normal eqns. When A is full-rank,
$\hat{b} = A(A^TA)^{-1}A^Tb$

Proof: a) $R(A^TA) = R(A^T) \longrightarrow$ Exercise

b) A full rank $\Rightarrow A^TA$ is non-singular
(Proof : exercise)

c) $R(A^TA) = R(A^T) \Leftrightarrow R(A^TA)^\perp = R(A^T)^\perp$

$\Leftrightarrow N(A^TA) = N(A)$

Hence $A^TA(\hat{x}_1 - \hat{x}_2) = 0 \Leftrightarrow A(\hat{x}_1 - \hat{x}_2) = 0$

d) From (c) $\hat{b}_1 = A\hat{x}_1$, $\hat{b}_2 = A\hat{x}_2$

$$(\hat{b}_1 - \hat{b}_2) = A(\hat{x}_1 - \hat{x}_2) = 0$$

Numerical Solution of Normal Eqns

If $x_{LS} = \arg\min_x \|Ax - b\|_2$ & $r_{LS} = b - Ax_{LS}$

then

Q1) How close is $\hat{x}_{LS}$ to x_{LS} ?

Q2) How close is $\hat{r}_{LS} := b - A\hat{x}_{LS}$ to r_{LS} ?

Cholesky Factorization (for full rank A)

Let $\text{rank}(A) = n$ || $A^T A x = \underbrace{A^T b}_{d}$

1) Compute $d = A^T b$

2) Compute $C = A^T A$ [$C > 0$, $\because$ A full rank]

3) Compute Cholesky factors of $C = GG^T$

4) Solve $\underset{\text{L.T.}}{G}y = d$ and $G^T x_{LS} = y$.

Algo requires $\left(m + \frac{n}{3}\right)n^2$ flops

B.E. : We know $(A^T A + E)\hat{x}_{LS} = A^T b$

where $\|E\| \approx cu\|A^T\|_2\|A\|_2 = cu\|A^T A\|_2$

↳ small constant

Then; $\left.\begin{array}{l} (A^T A + E)\hat{x}_{LS} = A^T b \\ A^T A x_{LS} = A^T b \end{array}\right]$ $A^T A\hat{x}_{LS} + E\hat{x}_{LS} - A^T A x_{LS} = 0$

$\Rightarrow A^T A[\hat{x}_{LS} - x_{LS}] = -E\hat{x}_{LS}$

$\Rightarrow \hat{x}_{LS} - x_{LS} = -(A^T A)^{-1} E\hat{x}_{LS}$

$$\|\hat{x}_{LS} - x_{LS}\| \leq \|(A^TA)^{-1}\| \|E\| \|\hat{x}_{LS}\|$$

as $$\frac{\|\hat{x}_{LS} - x_{LS}\|}{\|\hat{x}_{LS}\|} \lesssim \frac{cu\, \sigma_{max}(A^TA)}{\sigma_{min}(A^TA)}$$

$$\lesssim cu\, \kappa_2(A^TA) = cu\, \kappa_2^2(A)$$

Note: Fl. pt. errors in creating A^TA is ignored above. → can lead to serious errors.

L.S. solution via QR : Let $A = QR = Q\begin{bmatrix} R_1 \\ 0 \end{bmatrix}$ $(R_1 \in \mathbb{R}^{n\times n})$

Let $Q^Tb = \begin{array}{c} \begin{bmatrix} c \\ d \end{bmatrix} \end{array} \begin{array}{l} \}n \\ \}m-n \end{array}$

$$\|Ax-b\|_2^2 = \|Q^TAx - Q^Tb\|_2^2 = \|R_1x - c\|_2^2 + \|d\|_2^2$$

Hence $\underbrace{R_1 x_{LS} = c}_{\text{solve to get } x_{LS}}$ and $\|r_{LS}\|_2 = \|d\|_2$

Flops required : $2n^2(m - n/3)$ - same as Householder QR since $O(mn)$ for Q^Tb and $O(n^2)$ for back substitution are not significant.

Sensitivity of the Full Rank LS Problem (by QR)

Thm: Suppose that $x_{LS}, r_{LS}, \hat{x}_{LS}$ & $\hat{r}_{LS}$ satisfy

$$\|Ax_{LS} - b\|_2 = \min, \quad r_{LS} = b - Ax_{LS}$$

$$\|(A+\delta A)\hat{x}_{LS} - (b+\delta b)\|_2 = \min, \quad \hat{r}_{LS} = (b+\delta b) - (A+\delta A)\hat{x}_{LS}$$

where A has rank n and $\|\delta A\|_2 < \sigma_n(A)$.

Assume that b, r_{LS}, x_{LS} are not zero

Let $\theta_{LS} = (0, \pi/2)$ be defined by

$$\sin(\theta_{LS}) = \frac{\|r_{LS}\|_2}{\|b\|_2}$$

If $\varepsilon = \max\left\{\frac{\|\delta A\|_2}{\|A\|_2}, \frac{\|\delta b\|_2}{\|b\|_2}\right\}$ & $V_{LS} = \frac{\|A x_{LS}\|_2}{\sigma_n(A)\|x_{LS}\|_2}$

then:

$$\frac{\|\hat{x}_{LS} - x_{LS}\|_2}{\|x_{LS}\|_2} \leq \varepsilon\left\{\frac{V_{LS}}{\cos(\theta_{LS})} + \left[1 + V_{LS}\tan(\theta_{LS})\right]K_2(A)\right\} + O(\varepsilon^2)$$

$$\frac{\|\hat{r}_{LS} - r_{LS}\|_2}{\|r_{LS}\|_2} \leq \varepsilon\left\{\frac{1}{\sin\theta_{LS}} + \left[\frac{1}{V_{LS}\tan(\theta_{LS})} + 1\right]K_2(A)\right\} + O(\varepsilon^2)$$

Proof: Let $E = \frac{\delta A}{\varepsilon}$, $f = \frac{\delta b}{\varepsilon}$. Consider the solⁿ of

$$(A+tE)^T\underbrace{(A+tE)}_{\text{full rank } \forall t \in [0,\varepsilon]} x(t) = (A+tE)^T(b+tf) \quad \text{—— } (*)$$

$\# x_{LS} = x(0)$ and $\hat{x}_{LS} = x(\varepsilon)$. Hence

$$\hat{x}_{LS} = x_{LS} + \varepsilon\dot{x}(0) + O(\varepsilon^2)$$

$$\Rightarrow \frac{\|\hat{x}_{LS} - x_{LS}\|_2}{\|x_{LS}\|_2} = \varepsilon\frac{\|\dot{x}(0)\|_2}{\|x_{LS}\|_2} + O(\varepsilon^2) \quad \text{—— } (**)$$

Diff. $(*)$ at $t=0$ $\Big\}$, $\left[A^TA + tA^TE + tE^TA + t^2E^TE\right]x(t) = A^Tb + tE^Tb + tA^Tf + t^2E^Tf$

$$\left[A^TE + E^TA\right]x_{LS} + A^TA\dot{x}(0) = A^Tf + E^Tb$$

$$\Leftrightarrow \dot{x}(0) = [A^TA]^{-1}A^T[f - Ex_{LS}] + [A^TA]^{-1}E^Tr_{LS}$$

$$\|\dot{x}(0)\|_2 \leq \|[A^TA]^{-1}A^Tf\|_2 + \|[A^TA]^{-1}A^TEx_{LS}\|_2 + \|[A^TA]^{-1}E^Tr_{LS}\|_2$$

$$\leq \|(A^TA)^{-1}A^T\|_2\,\|\delta\|_2 + \|(A^TA)^{-1}A^T\|_2\,\|E\|_2\,\|x_{LS}\|_2 + \|(A^TA)^{-1}\|_2\,\|E\|_2\,\|r_{LS}\|_2$$

$$\leq \frac{\|b\|_2}{\sigma_n(A)} + \frac{\|A\|_2\|x_{LS}\|_2}{\sigma_n(A)} + \frac{\|A\|_2\|r_{LS}\|_2}{\sigma_n^2(A)}$$

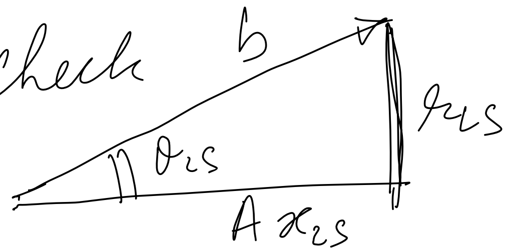
$$\left[\|(A^TA)^{-1}A^T\|_2 = \frac{1}{\sigma_n(A)}\ ;\ \|(A^TA)^{-1}\|_2 = \frac{1}{\sigma_n^2(A)}\ ;\ \|\delta\|\leq\|b\|,\ \|E\|\leq\|A\|\right]$$

Replacement in (**) yields:

$$\frac{\|\hat{x}_{LS}-x_{LS}\|}{\|x_{LS}\|} \leq \underbrace{\varepsilon\Bigg[\underbrace{\frac{\|b\|_2}{\sigma_n(A)\,\|x_{LS}\|_2}}_{(1)} + \underbrace{\frac{\|A\|_2}{\sigma_n(A)}}_{(2)} + \underbrace{\frac{\|A\|_2\|r_{LS}\|_2}{\sigma_n^2(A)\,\|x_{LS}\|}}_{(3)}\Bigg]}_{(*)} + O(\varepsilon^2)$$

Derivation of the r_{LS} bound is similar.

#Check



$$\sin(\theta_{LS}) = \frac{\|r_{LS}\|_2}{\|b\|_2}$$

$$\cos(\theta_{LS}) = \frac{\|Ax_{LS}\|}{\|b\|}$$

$$\tan(\theta_{LS}) = \frac{\|r_{LS}\|}{\|Ax_{LS}\|}\ ;\ \nu_{LS} = \frac{\|Ax_{LS}\|}{\sigma_n(A)\,\|x_{LS}\|_2} \leq \kappa_2(A)$$

Hence

$$(*) = \varepsilon\Bigg[\underbrace{\frac{\nu_{LS}}{\cos(\theta_{LS})}}_{(1)} + \underbrace{\kappa_2(A)}_{(2)} + \underbrace{\nu_{LS}\tan(\theta_{LS})\,\kappa_2(A)}_{(3)}\Bigg]$$

If $\left.\begin{array}{l}\cos(\theta_{LS}) \simeq 1\\ \Leftrightarrow \tan(\theta_{LS}) \simeq 0\end{array}\right\} \Rightarrow (*) \lesssim \varepsilon\left[\kappa_2(A) + \kappa_2(A)\right] \approx 2\varepsilon\,\kappa_2(A)$

\# QR is better when b is close to $\mathcal{R}(A)$.

QR Update

1) Rank 1 - Change : $A = QR$ known, $A \in \mathbb{R}^{n\times n}$

\# A is changed to $\tilde{A} = A + uv^T$. Compute $\tilde{A} = Q_1 R_1$

Clearly $\tilde{A} = A + uv^T = Q\left[R + wv^T\right]$

where $w = Q^T u$

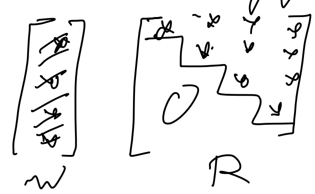
\# Use Givens rotations $J_{n-1}, \dots, J_2, J_1$ (each J_k in the plane $k, k+1$ to get

$$J_1^T \cdots J_{n-1}^T w = \pm \|w\|_2 e_1$$

\# Let $H = J_1^T \cdots J_{n-1}^T R$

Claim: H is upper Hessenberg

e.g.



$$J_3^T w = \begin{bmatrix} \times \\ \times \\ \times \\ 0 \end{bmatrix} \qquad J_3^T R = \begin{bmatrix} \times & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & 0 & \times & \times \\ 0 & 0 & \times & \times \end{bmatrix}$$

$$J_3^T = \left[\begin{array}{cc|cc} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \hline 0 & 0 & c & -s \\ 0 & 0 & s & c \end{array}\right]$$

$$\begin{bmatrix} c & -s \\ s & c \end{bmatrix}\begin{bmatrix} w_3 \\ w_4 \end{bmatrix} = \begin{bmatrix} w_3' \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} c & -s \\ s & c \end{bmatrix}\begin{bmatrix} r_{33} \\ 0 \end{bmatrix} = \begin{bmatrix} r_{33}' \\ r_{43}' \end{bmatrix} \to \text{non-zero likely}$$

Hence

$H =$ 

$\to$ upper Hessenberg

\# Then $\left[J_1^T \cdots J_{n-1}^T\right](R + wv^T) = H \pm \|w\|_2 e_1 v^T =: H_1$

is also upper Hessenberg

\# Convert H_1 to <u>upper triangular</u> by Givens rotations $G_{n-1}^T \cdots G_1^T H_1 = R_1$ ↳ upper triangular

Hence $\tilde{A} = A + uv^T = Q[R + wv^T]$

$$= Q[J_{n-1}\cdots J_1 H_1]$$

$$= \underbrace{[Q\,J_{n-1}\cdots J_1][G_1\cdots G_{n-1}]}_{Q_1} R_1 = Q_1 R_1$$

Flops required: $26n^2$
Compare a fresh QR: $\sim O(n^3)$

Exercise: Extend to $A \in \mathbb{R}^{m\times n}$

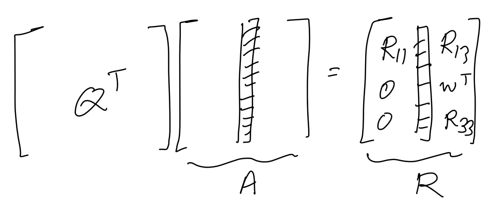
Deleting a Column

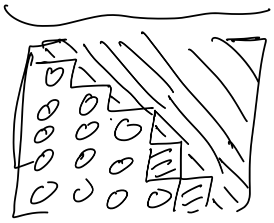
Let $QR = A = [a_1|\cdots|a_n]$ $\quad a_i \in \mathbb{R}^m$

$$R = \begin{array}{c c} \begin{bmatrix} R_{11} & v & R_{13} \\ 0 & r_{kk} & w^T \\ 0 & 0 & R_{33} \end{bmatrix} & \begin{array}{c} k-1 \\ 1 \\ m-k \end{array} \\ \begin{array}{ccc} k-1 & \quad 1 \quad & n-k \end{array} & \end{array}$$

Problem: Compute QR of $\tilde{A} = [a_1|\cdots|a_{k-1}|a_{k+1}|\cdots|a_n] \in \mathbb{R}^{m\times(n-1)}$

Then $Q^T\tilde{A} = \begin{bmatrix} R_{11} & R_{13} \\ 0 & w^T \\ 0 & R_{33} \end{bmatrix} =: H$ is upper Hessenberg





Construct $(n-k+1)$ Givens rotations s.t.
$G_{n-1}^T \cdots G_k^T H = R_1$ (upper triangular)

Then $\tilde{A} = Q^T H = \underbrace{Q^T(G_k \cdots G_{n-1})}_{Q_1} R_1$

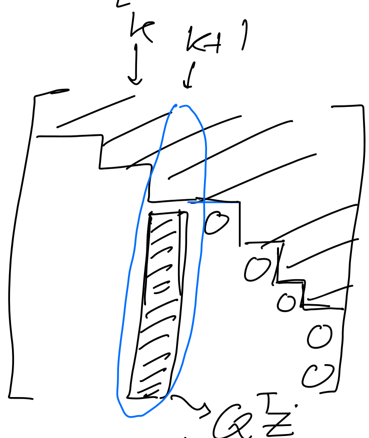
Flops $O(n^2)$ as compared to $O(n^3)$ for fresh QR

Appending a Column

Let $QR = A = [a_1 \cdots a_n]$. Add a column to A:

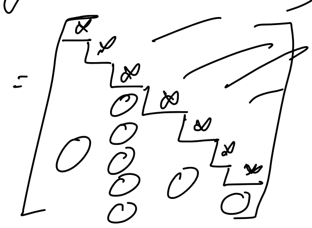
$$\tilde{A} = [a_1 \cdots a_k | z | a_{k+1} \cdots a_n] \in \mathbb{R}^{m\times(n+1)}$$

$Q^T\tilde{A} = [Q^Ta_1 \cdots Q^Ta_k | Q^Tz | Q^Ta_{k+1} \cdots Q^Ta_n]$



$= W$ (upper triangular except for $k+1^{th}$ col.)

$G_5 \cdots G_1 W =$



Use Givens rotation to zero out the spike:

$$G^T_{m-k-1} \cdots G_1^T W = R_1 \quad \text{upper triangular}$$

Then $\tilde{A} = QW = \underbrace{Q G_1 \cdots G_{m-k-1}}_{Q_1} R_1$

Adding a Row : Let $QR = A \in \mathbb{R}^{m\times n}$

QR Factorize $\tilde{A} = \begin{bmatrix} w^T \\ A \end{bmatrix}$, $w \in \mathbb{R}^n$

Clearly, $\left[\begin{array}{c|c} 1 & 0 \cdots 0 \\ \hline 0 & \\ \vdots & Q^T \\ 0 & \end{array}\right] \underbrace{\left[\begin{array}{c} w^T \\ \hline A \end{array}\right]}_{\tilde{A}} = \begin{bmatrix} w^T \\ R \end{bmatrix} = H$ (upper Hessenberg)

Determine Givens rotations $J_1, \cdots, J_n$ s.t.
$J_n^T \cdots J_1^T H = R_1$ is upper triangular

$\tilde{A} = \mathrm{diag}(1, Q) H = \underbrace{\mathrm{diag}(1, Q) J_1 \cdots J_n}_{Q_1} R_1$

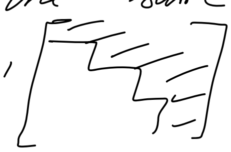
If $\tilde{A} = \begin{bmatrix} A_1 \\ w^T \\ A_2 \end{bmatrix}$ ($k+1^{th}$ row) & $\begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = QR$ is known, define $\tilde{A}_1 = \underbrace{\begin{bmatrix} 0 & 1 & 0 \\ I_k & 0 & 0 \\ 0 & 0 & I_{m-k} \end{bmatrix}}_{P} \tilde{A}$
$= \begin{bmatrix} w^T \\ A_1 \\ A_2 \end{bmatrix}$

Using previous method $\tilde{A}_1 = Q_1 R_1$,
then $\tilde{A} = \underbrace{P^T Q_1}_{Q_2} R_1$

<u>Deleting a Row</u>: $A = \begin{array}{c} \begin{bmatrix} z^T \\ A_1 \end{bmatrix} \begin{array}{l} 1 \\ m-1 \end{array} \end{array} = QR = \overbrace{\left[\begin{array}{c} q^T \\ \hline Z \end{array}\right]}^{Q} R$

Compute Givens rotations $G_1, \cdots, G_{m-1}$ s.t.
$G_1^T \cdots G_{m-1}^T q = \pm e_1$

If we apply the same G_i's on R,

$G_1^T \cdots G_{m-1}^T$  $=$  $=: \begin{bmatrix} v^T \\ R_1 \end{bmatrix} \begin{array}{l} 1 \\ m-1 \end{array}$

R $\qquad$ $H \to$ upper Hessenberg

upper triangular

Then $Q G_{m-1} \cdots G_1 = \begin{bmatrix} q^T \\ \hline Z \end{bmatrix} \underbrace{G_{m-1}}_{} \cdots G_1 = \left[\begin{array}{c|c} \pm 1 & 0 \cdots 0 \\ \hline 0 & \\ \vdots & Q_1 \\ 0 & \end{array}\right]$

orthogonal

$$\Rightarrow A = \begin{bmatrix} z^T \\ A_1 \end{bmatrix} = QR$$

$$= \left[Q G_{m-1} \cdots G_1 \right] \left[G_1^T \cdots G_{m-1}^T \ R \right]$$

$$= \begin{bmatrix} \pm 1 & 0 \\ 0 & Q_1 \end{bmatrix} \begin{bmatrix} v^T \\ R_1 \end{bmatrix}$$

$$\Rightarrow A_1 = Q_1 R_1$$

Q. What if A is not full rank?

Numerical Rank: $A = U \Sigma V^T$. If rank $A = r < n$, then $\sigma_{r+1} = \cdots = \sigma_n = 0$

$$A = \sum_{k=1}^{r} \sigma_k u_k v_k^T$$

However, computed numerically, $A = \sum_{k=1}^{n} \hat{\sigma}_k \hat{u}_k \hat{v}_k^T$

\# Choose a tolerance δ s.t.

$$\hat{\sigma}_1 \geq \cdots \geq \hat{\sigma}_{\hat{r}} > \delta \geq \hat{\sigma}_{\hat{r}+1} \geq \cdots \geq \hat{\sigma}_n$$

$\hat{r} \longrightarrow \delta$ - rank of A.

\# δ - is chosen usually as $\delta = u \|A\|_\infty$

QR with Column Pivoting: Modify Householder QR to get

$$Q^T A P = \begin{bmatrix} R_{11} & R_{12} \\ \underbrace{0}_{r} & \underbrace{0}_{n-r} \end{bmatrix} \begin{matrix} \} r = \text{rank}(A) \\ \} m - r \end{matrix}$$

R_{11}: u.T.

P: column permutation

If $AP = [a_{c_1} | \cdots | a_{c_n}]$, $Q = [q_1 \cdots q_m]$, then

$$a_{c_k} = \sum_{i=1}^{\min(r,k)} r_{ik} q_i \in \operatorname{span}\{q_1, \dots, q_r\} \quad \forall k = 1, \dots, n.$$

$$\operatorname{rank}(A) = \operatorname{span}\{q_1, \dots, q_r\}$$

for $j = 1:n$

$\quad c(j) = A(1:m, j)^T A(1:m, j)$

end

$\tau = \max\{c(1), \dots, c(n)\}$; $r = 0$

while $\tau > 0$ & $r < n$

$\quad r = r + 1$

$\quad$ Find smallest k $(r \le k \le n)$ s.t. $c(k) = \tau$

$\quad$ Permute r^{th} & k^{th} columns of A

$\quad [v, \beta] = \operatorname{house}(A(r:m, r))$

Usual H. QR after col. pivoting

$\quad A(r:m, r:n) = (I_{m-r+1} - \beta v v^T) A(r:m, r:n)$

$\quad A(r+1:m, r) = v(2:m-r+1)$

$\quad$ for $i = r+1 : n$

$\quad\quad c(i) = c(i) - A^2(r, i)$

$\quad$ end

$\quad \tau = \max\{c(r+1), \dots, c(n)\}$

end

Normally one would require to recompute

$$c(j) = A(1:m, j)^T A(1:m, j) \quad \text{for } j = k+1 : n$$

after k^{th} step.

However $\quad Q^T z = \begin{bmatrix} \alpha \\ w \end{bmatrix} \Rightarrow \|w\|_2^2 = \|z\|_2^2 - \alpha^2$

Hence the new $c(j)$'s can be computed directly by subtraction of $A^2(r,i)$

Q. Does the above method reveal numerical rank?

$$fl(H_k \cdots H_1 A P_1 \cdots P_k) = \begin{array}{cc} \left[\begin{array}{cc} \hat{R}_{11}^{(k)} & \hat{R}_{12}^{(k)} \\ O & \hat{R}_{22}^{(k)} \end{array}\right] & \begin{array}{c} k \\ m-k \end{array} \\ \begin{array}{cc} k & n-k \end{array} & \end{array}$$

\# If $\|\hat{R}_{22}^{(k)}\|_2 \le \underbrace{\varepsilon_1}_{\text{some machine dependent parameter}} \|A\|_2$ we can claim that numerical rank of $A = k$. (Converse however is not always true Golub pg. 279)

Basic Solution of LS with QR with Column Pivoting

$$AP = QR = Q \begin{array}{cc} \left[\begin{array}{cc} R_{11} & R_{12} \\ O & O \end{array}\right] & \begin{array}{c} r \\ n-r \end{array} \\ \begin{array}{cc} r & n-r \end{array} & \end{array}$$

$$\|Ax - B\|_2^2 = \|(Q^T A P)(P^T x) - Q^T b\|_2^2 \qquad \left| \; Q^T b = \begin{bmatrix} c \\ d \end{bmatrix} \begin{array}{c} r \\ m-r \end{array} \right.$$

$$= \|R_{11} y - (c - R_{12} z)\|_2^2 + d^2 \qquad \left| \; P^T x = \begin{bmatrix} y \\ z \end{bmatrix} \begin{array}{c} r \\ n-r \end{array} \right.$$

$$\Rightarrow \quad x^* = P \begin{bmatrix} R_{11}^{-1}(c - R_{12} z) \\ z \end{bmatrix} \quad \text{---} (*)$$

\# For each z, we have a different sol^n x^*.
For $z = 0$, $x_B := P \begin{bmatrix} R_{11}^{-1} c \\ 0 \end{bmatrix} \leftarrow$ Basic sol^n

A more careful analysis of Rank deficient LS requires SVD.

The minimum norm sol$\underline{\underline{n}}$:

FACT: The set of all minizers for the L.S. problem: $\mathcal{X} = \{x \in \mathbb{R}^n : \|Ax-b\|_2 = \min\}$ is convex.

Proof: If $x_1, x_2 \in \mathcal{X}$ and $\lambda \in [0,1]$, then

$$\|A(\lambda x_1 + (1-\lambda)x_2) - b\|_2$$
$$\leq \lambda\|Ax_1 - b\|_2 + (1-\lambda)\|Ax_2 - b\|_2$$
$$= \min_{x \in \mathbb{R}^n} \|Ax - b\|_2$$
$$\Rightarrow [\lambda x_1 + (1-\lambda)x_2] \in \mathcal{X}$$

FACT: $\exists$ unique $x_{LS} \in \mathcal{X}$ s.t. $\|x_{LS}\|_2 = \min \|x\|_2 \ \forall x \in \mathcal{X}$.

(Recall in full-rank case there is only one x_{LS})

FACT: Let $A = U\Sigma V^T$, $A \in \mathbb{R}^{m\times n}$ with rank $(A) = r$. $U = [u_1 \cdots u_m]$ & $V = [v_1 \cdots v_n]$, & $b \in \mathbb{R}^m$

Then $$x_{LS} = \sum_{i=1}^{r} \frac{u_i^T b}{\sigma_i} v_i$$

Moreover, $$\rho_{LS}^2 = \|Ax_{LS} - b\|^2 = \sum_{i=r+1}^{m} (u_i^T b)^2$$

Proof: $\|Ax-b\|_2^2 = \|(U^TAV)(\underbrace{V^Tx}_{\alpha}) - U^Tb\|_2^2$ $\quad \boxed{\alpha = V^Tx}$

$= \|\Sigma\alpha - U^Tb\|_2 = \sum_{i=1}^{r}(\sigma_i\alpha_i - u_i^Tb)^2 + \sum_{i=r+1}^{m}(u_i^Tb)^2$

$\Rightarrow$ Min 2-norm solution $\left.\right\}$ $\alpha_i = \begin{cases} \dfrac{u_i^Tb}{\sigma_i}, & i=1\cdots r \\ 0 & i=r+1,\cdots,n \end{cases}$

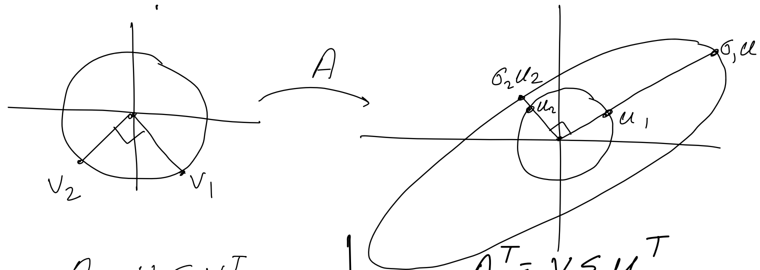
$0 \to$ choose.

$x_{LS} = V\alpha$

$\|x_{LS}\|_2 = \|\alpha\|_2$

Recall Geometry of SVD:

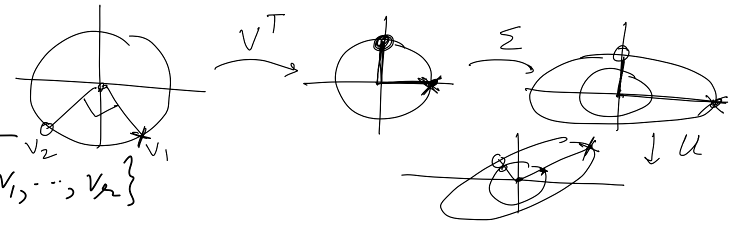
$$\begin{array}{l} v_1 \xrightarrow[A]{\sigma_1} u_1 \xrightarrow[A^T]{\sigma_1} v_1 \\ v_2 \xrightarrow{\sigma_2} u_2 \xrightarrow{\sigma_2} v_2 \\ \vdots \\ v_r \xrightarrow{\sigma_r} u_r \xrightarrow{\sigma_r} v_r \\ \left.\begin{array}{l} v_{r+1} \\ \vdots \\ v_m \end{array}\right\} \to 0 \quad \left.\begin{array}{l} u_{r+1} \\ \vdots \\ u_n \end{array}\right\} \to 0 \end{array}$$



$A = U\Sigma V^T$ $\quad A^T = V\Sigma U^T$

or $AV = U\Sigma$

$[Av_1 \ \ Av_2] = [u_1 \ \ u_2]\begin{bmatrix}\sigma_1 & 0 \\ 0 & \sigma_2\end{bmatrix} = [\sigma_1 u_1 \ \ \sigma_2 u_2]$



Recall

$R(A) = sp\{u_1,\cdots,u_r\}$	$R(A^T) = sp\{v_1,\cdots,v_r\}$
$N(A) = sp\{v_{r+1},\cdots,v_n\}$	$N(A^T) = sp\{u_{r+1},\cdots,u_m\}$

Pseudo-inverse $\to$ almost like inverse

$$\begin{array}{l} u_1 \xrightarrow[A^+]{\sigma_1^{-1}} v_1 \\ u_2 \xrightarrow{\sigma_2^{-1}} v_2 \\ \vdots \\ u_r \xrightarrow{\sigma_r^{-1}} v_r \\ \left.\begin{array}{l} u_{r+1} \\ \vdots \\ u_n \end{array}\right\} \to 0 \end{array}$$

rank(A^+) = rank(A)

The top parts:

$$\left.\begin{array}{l} v_1 \xrightarrow[{[A]_r}]{\sigma_1} u_1 \xrightarrow[{[A^+]_r}]{\sigma_1^{-1}} v_1 \\ \vdots \\ v_r \xrightarrow{\sigma_r} u_r \xrightarrow{\sigma_r^{-1}} v_r \end{array}\right\}$$ True inverses of each other

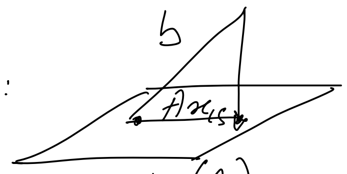
Pseudo-Inverse : $A^+ = V\Sigma^+ U^T \in \mathbb{R}^{n\times m}$

$$\Sigma^+ = \mathrm{diag}\left(\frac{1}{\sigma_1}, \dots, \frac{1}{\sigma_r}, 0, \dots, 0\right) \in \mathbb{R}^{n\times m}$$

Then: $x_{LS} = A^+ b$ & $\rho_{LS} = \| [I - AA^+] b \|_2$

If $\mathrm{rank}(A) = n$ then $A^+ = (A^TA)^{-1}A^T$
If $m = n = \mathrm{rank}(A)$ the $A^+ = A^{-1}$

Projections :



$Ax_{LS} = \underbrace{AA^+}b$
orthogonal projection matrix
$\rightarrow$ projecting b onto $R(A)$

Check this projection property
P, is an orthogal projection if $P^2 = P = P^T$ clearly satisfies

$AA^+ = U_1 U_1^T$
$A^+A = V_1 V_1^T$

$U_1 = U(1:m, 1:r)$
$V_1 = V(1:n, 1:r)$

Recall
$R(A) = \mathrm{sp}\{u_1, \dots, u_r\}$
$N(A) = \mathrm{sp}\{v_{r+1}, \dots, v_n\}$
$R(A^T) = \mathrm{sp}\{v_1, \dots, v_r\}$
$N(A^T) = \mathrm{sp}\{u_{r+1}, \dots, u_m\}$

$$\Rightarrow [AA^+]\underset{\mathbb{R}^m}{x} = \underset{m\times r}{U_1}\underset{r\times m}{U_1^T} x \in \mathrm{sp}\{u_1, \dots, u_r\} = R(A)$$

$\hookrightarrow$ orthogonal projection onto $R(A)$

$$\Rightarrow [A^+A]y = [\underset{n\times r}{V_1}\underset{r\times n}{V_1^T}]\underset{\mathbb{R}^n}{y} \in \mathrm{sp}\{v_1, \dots, v_r\} = R(A^T)$$

$\hookrightarrow$ orthogonal projection onto $R(A^T)$

Exercise: Check A^+ satisfies the four Moore-Penrose conditions:
(i) $AXA = A$
(ii) $XAX = X$
(iii) $(AX)^T = AX$
(iv) $(XA)^T = XA$

Underdetermined Linear Systems

$A \in \mathbb{R}^{m\times n}$, $m<n$. $\text{rank}(A)=m$, $b \in \mathbb{R}^m$

solve $Ax=b$

$$\begin{bmatrix} & A & \end{bmatrix}\begin{bmatrix} \\ x \\ \\ \end{bmatrix} = \begin{bmatrix} b \end{bmatrix}$$

Infinitely many solutions.

Q. Can we use LU to solve for at least one of the solutions?

Q. Can we use QR to find the min-norm soln.?

LU with Complete / Rook Pivoting

$PAQ^T = L[U_1 \mid U_2]$ $\quad U_1 \in \mathbb{R}^{m\times m}$ non-singular and upper tr.

L: $\mathbb{R}^{m\times m}$ unit lower triangular $\quad U_2 \in \mathbb{R}$

$$\underbrace{\underset{m\times m}{[P]}\underset{m\times n}{\begin{bmatrix} & A & \end{bmatrix}}\underset{n\times n}{\begin{bmatrix} & & \\ & Q^T & \\ & & \end{bmatrix}}}_{m\times n} = \underset{m\times m}{\underset{L}{[\;]}}\;\underset{m\times m}{\underset{U_1}{[\;}}\;\underset{m\times(n-m)}{\underset{U_2}{\;]}}$$

$$Ax=b \iff \left(PAQ^T\right)(Qx) = Pb$$

$$\iff L[U_1 \mid U_2]\begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = L\left(U_1 z_1 + U_2 z_2\right) = c$$

where $Qx = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$ and $c = Pb$

1) Solve $Ly = Pb$ $\longrightarrow$ $z_2 = 0$ is a natural choice
2) Choose $z_2 \in \mathbb{R}^{n-m}$ & solve $U_1 z_1 = y - U_2 z_2$ for z_1
3) Set $x = Q^T \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$.

QR can find the min-norm sol$^{\underline{n}}$

Assume A has full row rank $= m$ (as above)

$$Q^T A P = [R_1 \;\; R_2] \leftarrow \text{QR with col pivoting}$$

$$\underbrace{\underset{m\times m}{[Q^T]}\underset{m\times n}{[\;A\;]}\underset{n\times n}{\begin{bmatrix} \\ P \\ \\ \end{bmatrix}}}_{m\times n} = [\underset{m\times m}{\underbrace{R_1}}\;\; \underset{m\times(n-m)}{R_2}]$$

If $Ax = b$, $(Q^T A P)(\underbrace{P^T x}_{\substack{\mathbb{R}^m \leftarrow z_1 \\ \mathbb{R}^{n-m} \leftarrow z_2}}) = [R_1 \;\; R_2]\begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = Q^T b$

Due to col. pivoting, R_1 is non-singular ($\because A$ has full rank)

One sol$^{\underline{n}}$: $z_2 = 0$, $z_1 = R_1^{-1} Q^T b$, $x = P\begin{bmatrix} z_1 \\ 0 \end{bmatrix}$
However min-norm is not guaranteed. $\|z_1\|_2$ depends on choice of P.

Flops: $2m^2 n - \frac{m^3}{3}$ (Exercise)

Alternatively, compute $A^T = QR = Q\begin{bmatrix} R_1 \\ 0 \end{bmatrix}$ $\} m\times m$
Then $Ax = b \Rightarrow (QR)^T x = R^T Q^T x$

$$= [R_1 \,|\, 0]\,[\underbrace{Q^T x}] = [R_1 \,|\, 0]\begin{bmatrix} z_1 \\ \hline z_2 \end{bmatrix} = b$$

$$z = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \begin{array}{l} \to m \\ \to n-m \end{array}$$

\# Put $z_2 = 0$, $z_1 = R_1^{-1} b$ $\leftarrow$ min $\|\cdot\|_2$ norm soln.

\# Flops: $2m^2 n - \dfrac{2m^3}{3}$ (Exercise)

<u>SVD</u>: SVD can be used exactly as in the over determined case:

<u>Min Norm soln</u> to $Ax = b$

$$\underset{m\times n}{\begin{bmatrix} & A & \end{bmatrix}} = \underset{m\times m}{[U]}\ \underbrace{\begin{bmatrix} \underbrace{\ddots}_{r}\ \ \ \ \ \ & \Big| & \underbrace{0}_{n-m} \end{bmatrix}}_{\underbrace{\qquad m \qquad}_{\Sigma}} \underset{n\times n}{\begin{bmatrix} & & \\ & V^T & \\ & & \end{bmatrix}}$$

$$A = \sum_{i=1}^{r} \sigma_i u_i v_i^T$$

$$x^* = \sum_{i=1}^{r} \frac{u_i^T b}{\sigma_i} v_i$$

<u>Comparison for Square System</u>

LU $\longrightarrow \dfrac{2n^3}{3}$

Householder QR $\longrightarrow 4n^3/3$

MGS $\longrightarrow 2n^3$

SVD $\longrightarrow 12n^3$