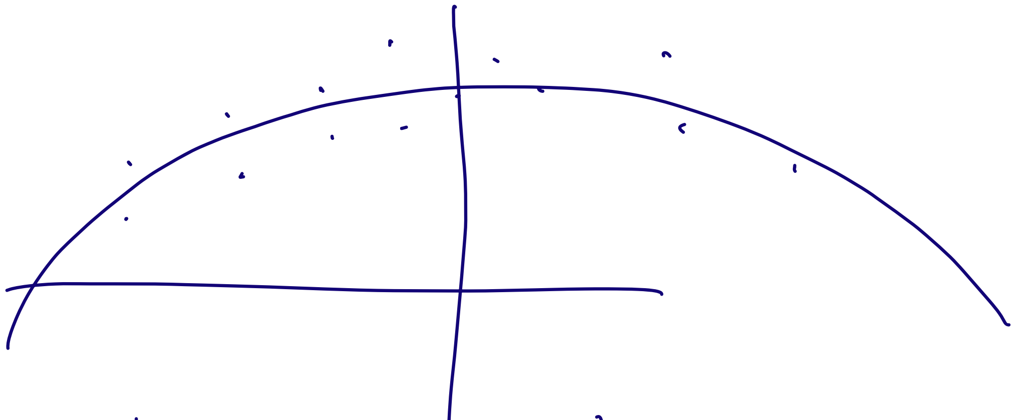
Least Squares



overdetermined systems

$A = \begin{pmatrix} \\ \\ \\ \end{pmatrix}$ $\qquad \underbrace{Ax \approx b}$

$$\boxed{\min \| b - Ax \|_2^2}$$

normal equations $\qquad \underline{A^T A} x = A^T \underline{b}$

if $A^T A$ invertible $\qquad x = (A^T A)^{-1} A^T b$

$m > n$ $\qquad \Updownarrow$ rank$(A) = n$

QR decomposition

$$\underset{m\times n}{A} = \underset{m\times m}{Q}\ \underset{m\times n}{R}$$

$$= \begin{array}{cc} \begin{pmatrix} Q_1 & Q_2 \end{pmatrix} \\ \begin{array}{cc} \underline{n} & \underline{m-n} \end{array} \end{array} \begin{array}{c} n \\ \begin{pmatrix} \hat{R} \\ O \end{pmatrix} \end{array} \begin{array}{c} \underline{n} \\ \underline{m-n} \end{array} = Q_1\hat{R} + Q_2 O$$

$$= Q_1\hat{R}$$

$$\begin{array}{cc} & 2 \\ 10 & \begin{pmatrix} | & | \\ a_1 & a_2 \\ | & | \end{pmatrix} \end{array} = \begin{pmatrix} | & | \\ q_1 & q_2 \\ | & | \end{pmatrix} \underset{2\times 2}{\begin{pmatrix} r_{11} & r_{12} \\ & r_{22} \end{pmatrix}}$$

$$10\times 2$$

$$\begin{array}{cc} Q_1 & Q_2 \\ \begin{pmatrix} | & | \\ q_1 & q_2 \\ | & | \end{pmatrix} & \begin{pmatrix} | & & | \\ q_3 & \cdots & q_{10} \\ | & & | \end{pmatrix} \end{array} \begin{pmatrix} r_{11} & r_{12} \\ & r_{22} \\ 0 & 0 \\ \vdots & \\ 0 & 0 \end{pmatrix}$$

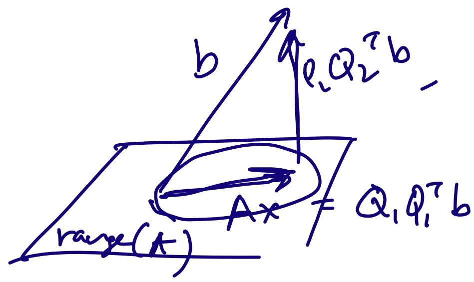
$$Q$$

$$QR = \left(Q_1 \,\middle|\, Q_2\right)\begin{pmatrix}\hat{R}\\ 0\end{pmatrix}$$

Find x that minimizes

$$\|b - Ax\|_2^2 \qquad\qquad \|y\|_2 = \|Qy\|_2$$

$$= \|\boxed{b - QRx}\|_2^2$$



multiply by Q^T

$$= \|Q^Tb - \cancel{Q^TQ}Rx\|_2^2$$

$$= \|Q^Tb - Rx\|_2^2 \qquad = \left\langle QR = (Q_1|Q_2)\begin{pmatrix}\hat{R}\\ 0\end{pmatrix}\right\rangle$$

$$= \left\|\begin{pmatrix}Q_1^Tb\\ Q_2^Tb\end{pmatrix} - \begin{pmatrix}\hat{R}x\\ 0\end{pmatrix}\right\|_2^2$$

$$= \left\|\begin{matrix}\boxed{Q_1^Tb - \hat{R}x}\\ \boxed{Q_2^Tb - 0}\end{matrix}\right\|_2^2$$

$$\left\|\begin{pmatrix}x_1\\ x_2\end{pmatrix}\right\|_2^2 = x_1^2 + x_2^2$$

$$\left\|\begin{pmatrix}x\\ y\\ z\end{pmatrix}\right\|_2^2 = \left\|\begin{pmatrix}x\\ y\end{pmatrix}\right\|_2^2 + \|(z)\|_2^2$$

$$= \underbrace{\boxed{\overset{=0}{\|Q_1^T b - \hat{R}x\|_2^2}}}_{\text{Solve by back subst.}} + \|Q_2^T b\|_2^2 = \|r\|_2^2$$

$$\boxed{\hat{R}x = Q_1^T b}$$

$\Sigma^T \Sigma$

if $\hat{R}$ invertible $\Longleftrightarrow$ $\boxed{A^T A}$ invertible

$$\boxed{x = \hat{R}^{-1} Q_1^T b}$$

$\mathrm{cond}(A^T A) = \mathrm{cond}(A)^2$

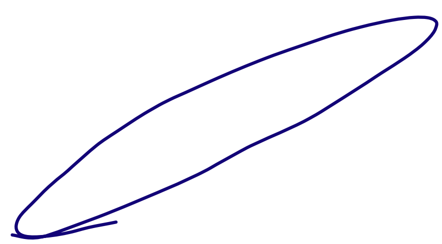
$$\mathrm{cond}_2(A) = \|A\|_2 \|A^{-1}\|_2$$

smallest σ of A: σ_n

$$\|A\|_2 = \sigma_1$$

largest σ of A^{-1} $\quad \frac{1}{\sigma_n}$

$$\mathrm{cond}_2(A) = \frac{\sigma_1}{\sigma_n}$$



$$A = QR$$

$$U \Sigma V^T = \boxed{QR}$$

$$\underbrace{QU}\Sigma V^T$$

multiplying by Q doesn't change Σ in the SVD

$$(Q^T U)\boxed{\Sigma} V^T = R$$

$$\text{cond}_2(A) = \text{cond}_2(R)$$

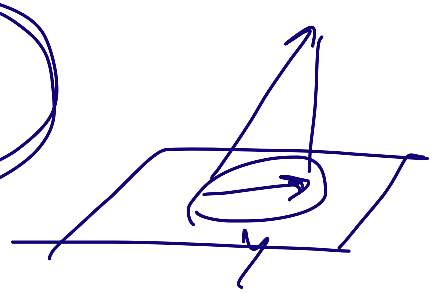
A <u>not</u> full rank $\iff \exists\, z \neq 0 \quad Az = 0$

using <u>SVD</u> to solve L.S. problem

$$y = A\boxed{x + \alpha z}$$

many solutions possible

$$\|x + \alpha z\|_2^2$$



<u>minimum norm</u> solution

$m > n$

$$\underset{m\times n}{A} = \underset{m\times m}{U}\,\underset{m\times n}{\Sigma}\,\underset{n\times n}{V^T}$$

$\text{rank}(A) = r < n$

$$A = \begin{pmatrix} U_1 & \Big| & U_2 \end{pmatrix} \begin{array}{cc} r & n-r \\ \left[\begin{array}{c|c} \begin{matrix}\sigma_1 & & \\ & \ddots & \\ & & \sigma_r \end{matrix} & \begin{matrix} 0 & & \\ & \ddots & \\ & & 0\end{matrix} \end{array}\right] & \end{array} \begin{array}{c} \begin{bmatrix} V_1^T \\ V_2^T \end{bmatrix} \end{array} \begin{array}{c} r \\ n-r \end{array}$$

find x^* that $\quad r \quad m-r$

$$\min \| b - Ax \|_2^2$$

$$\boxed{x^* = \underset{x}{\operatorname{argmin}} \underbrace{\| b - Ax \|_2^2}}$$

$$= \| \underbrace{b - U \Sigma V^T x} \|_2^2$$

$$= \| U^T b - \Sigma V^T x \|_2^2$$

$$= \left\| \begin{pmatrix} U_1^T b \\ U_2^T b \end{pmatrix} - \begin{pmatrix} \Sigma_1 & 0 \end{pmatrix} \begin{pmatrix} V_1^T x \\ V_2^T x \end{pmatrix} \right\|_2^2$$

$$= \left\| \begin{pmatrix} U_1^T b \\ U_2^T b \end{pmatrix} - \begin{pmatrix} \Sigma_1 V_1^T x \\ 0 \end{pmatrix} \right\|_2^2$$

$$= \underbrace{\| U_1^T b - \Sigma_1 V_1^T x \|_2^2} - \underbrace{\| U_2^T b - 0 \|_2^2}$$

$$\Rightarrow \quad U_1^T b = \Sigma_1 V_1^T x$$

$$\boxed{V_1^T x = \Sigma_1^{-1} U_1^T b}$$

$$V_2^T x = \; ?$$

V_2 basis for the nullspace of A

$$\left(U_1 \middle| U_2\right) \Sigma \begin{pmatrix} V_1 \\ \hline \boxed{V_2} \end{pmatrix}$$

min. norm solution:

$$\underline{V_2^T x} = 0$$

$$\boxed{V_1^T x = \Sigma_1^{-1} U_1^T b}$$

$$v_i^T x = \frac{1}{\sigma_i} u_i^T b \quad \text{for } i = 1, \dots, r$$

$$\boxed{x = \sum_{i=1}^{r} \underbrace{\left(\frac{1}{\sigma_i} u_i^T b\right)}\, v_i}$$

minimum norm solution

$$v_1^T x = \alpha_1 \qquad \|v_1\|_2 = 1$$

$$x = \alpha_1 v_1$$

$$\vec{x}$$

$\{q_1, \dots, q_n\}$ orthonormal basis

$$\underline{\vec{x}} = \underline{q_1^T x}\, \underline{q_1} + \dots + \underline{q_n^T x}\, q_n$$

$$\|x\|_2^2 = (q_1^T x)^2 + \dots + (q_n^T x)^2$$

$$e_1, \dots, e_n$$

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pseudoinverse of A

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

if A invertible

$$A^{-1} = V \Sigma^{-1} U^T$$

if A not invertible

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

$$\Sigma^{+} = \begin{pmatrix} \frac{1}{\sigma_1} & & & & & \\ & \ddots & & & & \\ & & \frac{1}{\sigma_r} & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \end{pmatrix}$$

$$\Sigma^{+}_{ii} = \begin{cases} \frac{1}{\sigma_i} & \text{if } \sigma_i > 0 \\ 0 & \text{if } \sigma_i = 0 \end{cases}$$

$$A = U \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_r \end{pmatrix} V^T$$

$$A^{-1} = V \begin{pmatrix} \frac{1}{\sigma_1} & & \\ & \ddots & \\ & & \boxed{\frac{1}{\sigma_r}} \end{pmatrix} U^T$$

$$A^{+} = V \begin{pmatrix} \frac{1}{\sigma_1} & & & \\ & \ddots & & \\ & & \frac{1}{\sigma_{r-1}} & \\ & & & 0 \end{pmatrix} U^T$$

$$\boxed{x = \underbrace{\sum_{i=1}^{r} \left(\frac{1}{\sigma_i} u_i^T b\right) v_i}} = \underbrace{A^+ b}$$

$$x = A^+ b \qquad U \Sigma V^T$$

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

$$A^+ b = V \Sigma^+ U^T b$$

$$= \begin{pmatrix} v_1 & v_2 \end{pmatrix} \begin{pmatrix} \hat{\Sigma}^{-1} & 0 \end{pmatrix} \begin{pmatrix} u_1^T \\ u_2^T \end{pmatrix} b$$

$$= \begin{pmatrix} v_1 & v_2 \end{pmatrix} \begin{pmatrix} \hat{\Sigma}^{-1} & 0 \end{pmatrix} \begin{pmatrix} u_1^T b \\ u_2^T b \end{pmatrix}$$

$$\boxed{A^+ b = V_1 \hat{\Sigma}^{-1} U_1^T b}$$