COL 726: Solving linear systems w/ QR
least squares problems.

$A = \hat{Q}\hat{R} = QR$

$A\vec{x} = \vec{b}$: solve

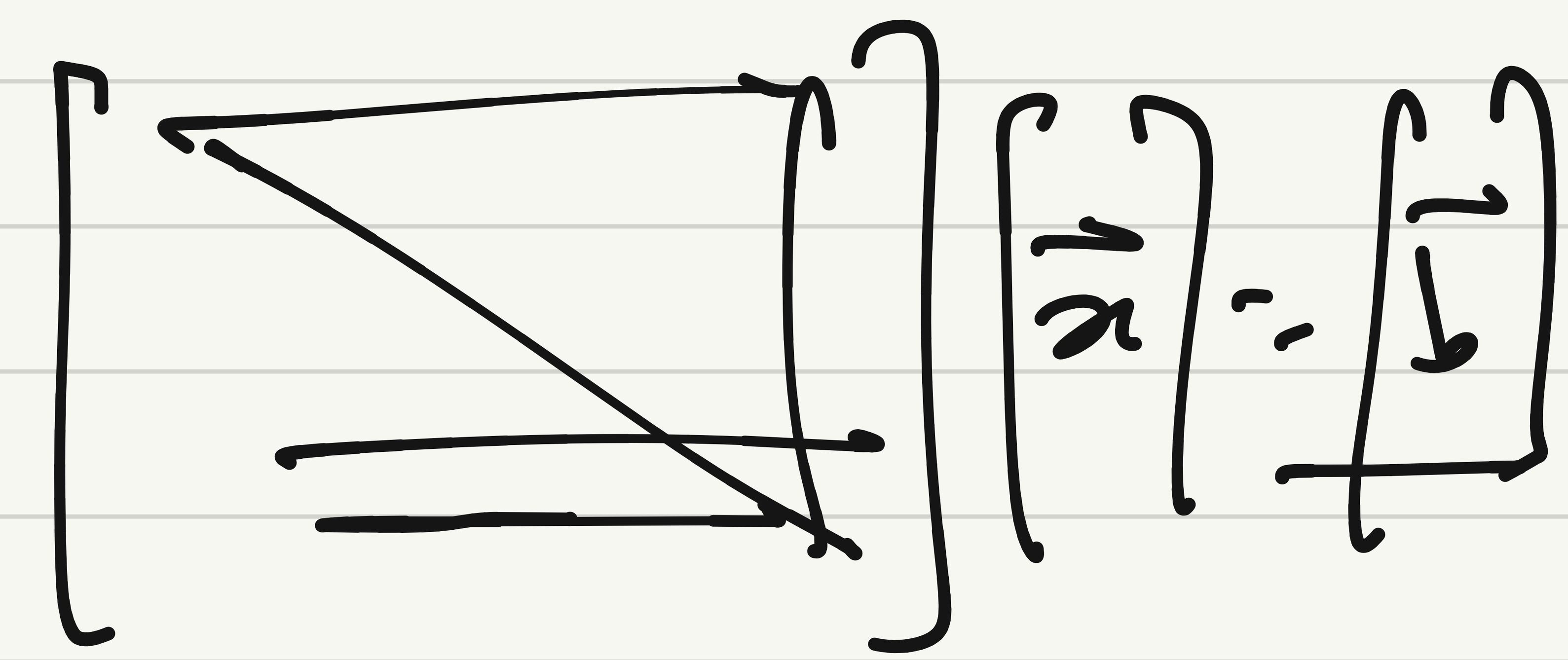
$QR\vec{x} = \vec{b}$

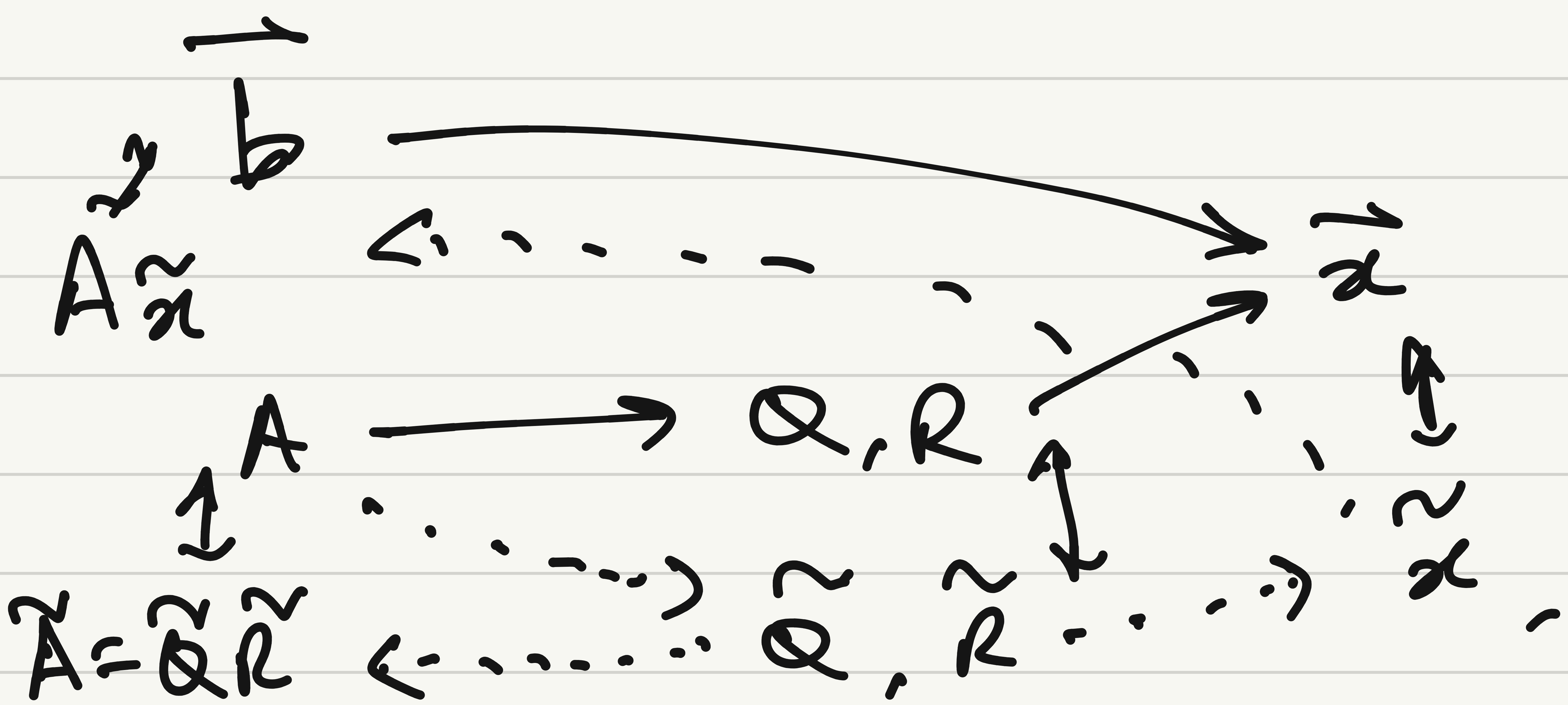
$R\vec{x} = \underbrace{Q^*\vec{b}}_{\vec{w}}$

① $Q, R = \text{house}(A)$

② $\vec{w} = Q^*\vec{b}$

③ $\vec{x} = R^{-1}\vec{w}$


backsub.



random $R \in \mathbb{R}^{50\times50}$

random $Q \in \mathbb{R}^{50\times50}$

$\|\tilde{x} - x\|$

$A = QR$

$\tilde{Q}, \tilde{R} = \text{house}(A)$

$\|\tilde{Q} - Q\|, \quad \dfrac{\|\tilde{R} - R\|}{\|R\|} \approx 10^{-2}$

$\dfrac{\|A\tilde{x} - \vec{b}\|}{\|\vec{b}\|} = O(\varepsilon_m)$

Householder QR is not accurate but is backward stable!

Thm. $\dfrac{\|\tilde{Q}\tilde{R}-A\|}{\|A\|} = O(\varepsilon_{machine})$

$\vec{v}_1, \vec{v}_2, \ldots, \vec{v}_n$

$\Rightarrow \tilde{Q}\tilde{R} = A + \delta A$ with $\dfrac{\|\delta A\|}{\|A\|} = O(\varepsilon_m)$

$A\vec{x} = \vec{b}$

$\vec{w} = Q^*\vec{b}$, $\vec{x} = R^{-1}\vec{w}$

$(A+\Delta A)\tilde{x} = \vec{b}$

$(\tilde{Q} + \delta\tilde{Q})\tilde{w} = b$ $\qquad \|\delta\tilde{Q}\| = O(\varepsilon_m)$

$\dfrac{\|\vec{x} - \tilde{x}\|}{\|\vec{x}\|} = O(K(A)\varepsilon_m)$

$(\tilde{R} + \delta\tilde{R})\tilde{x} = \tilde{w}$ $\qquad \dfrac{\|\delta\tilde{R}\|}{\|\tilde{R}\|} = O(\varepsilon_m)$

$A + \delta A$

$\vec{b} = (\tilde{Q} + \delta\tilde{Q})(\tilde{R} + \delta\tilde{R})\tilde{x} = \underbrace{(\tilde{Q}\tilde{R} + \delta\tilde{Q}\tilde{R} + \tilde{Q}\delta\tilde{R} + \delta\tilde{Q}\delta\tilde{R})}_{A + (\Delta A)}\tilde{x}$

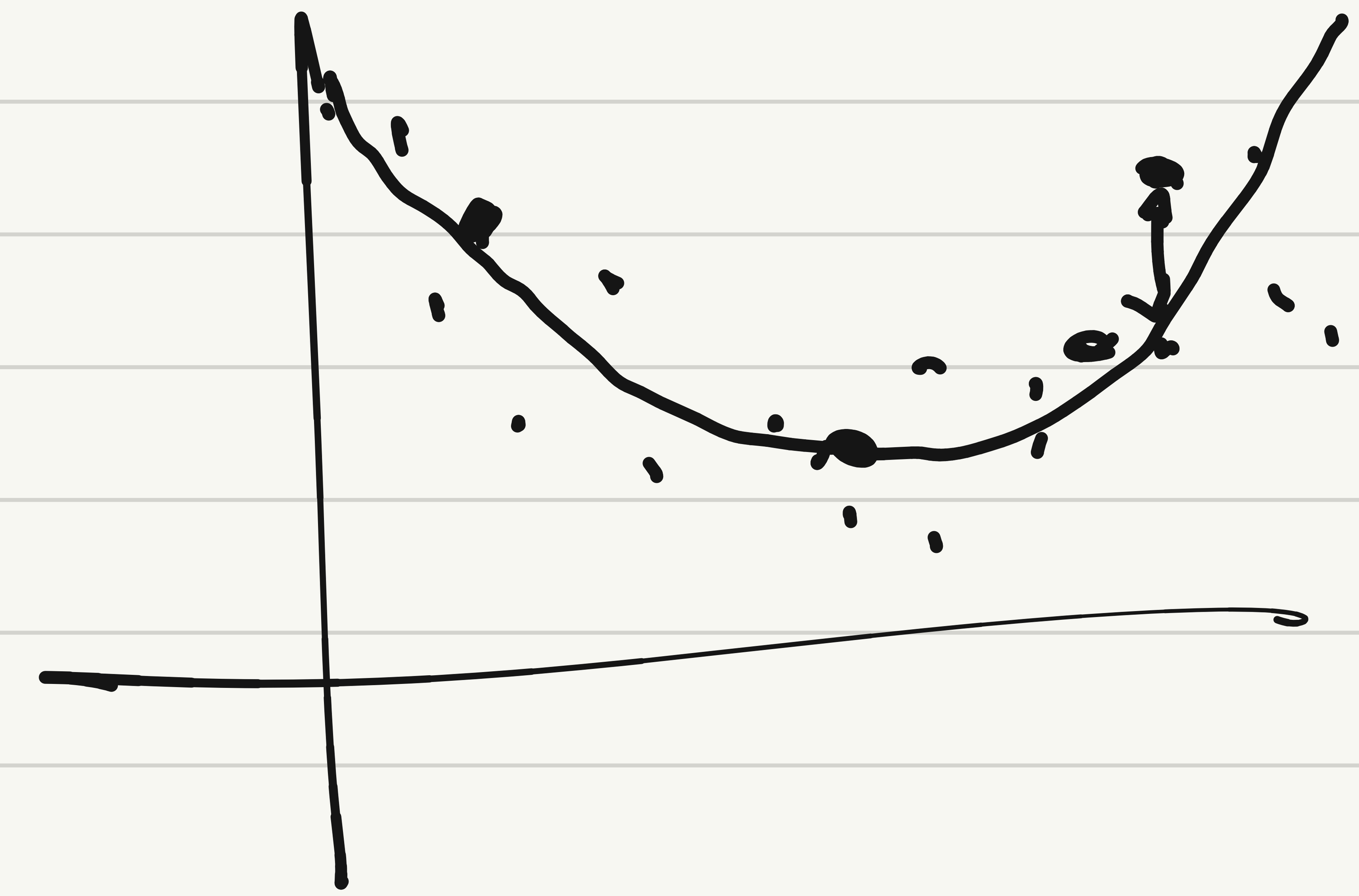
$A + (\Delta A) \rightarrow \dfrac{\|\Delta A\|}{\|A\|} = O(\varepsilon_m)$

least-squares problems

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

$\text{range}(A) \subset \mathbb{C}^m$

$\vec{b} \notin \text{range}(A)$



$A \in \mathbb{C}^{m \times n}$ full rank.

$m > n$

$$\begin{bmatrix} x_1^2 & x_1 & 1 \\ x_1^2 & x_2 & 1 \\ \vdots & \vdots & \vdots \end{bmatrix}$$

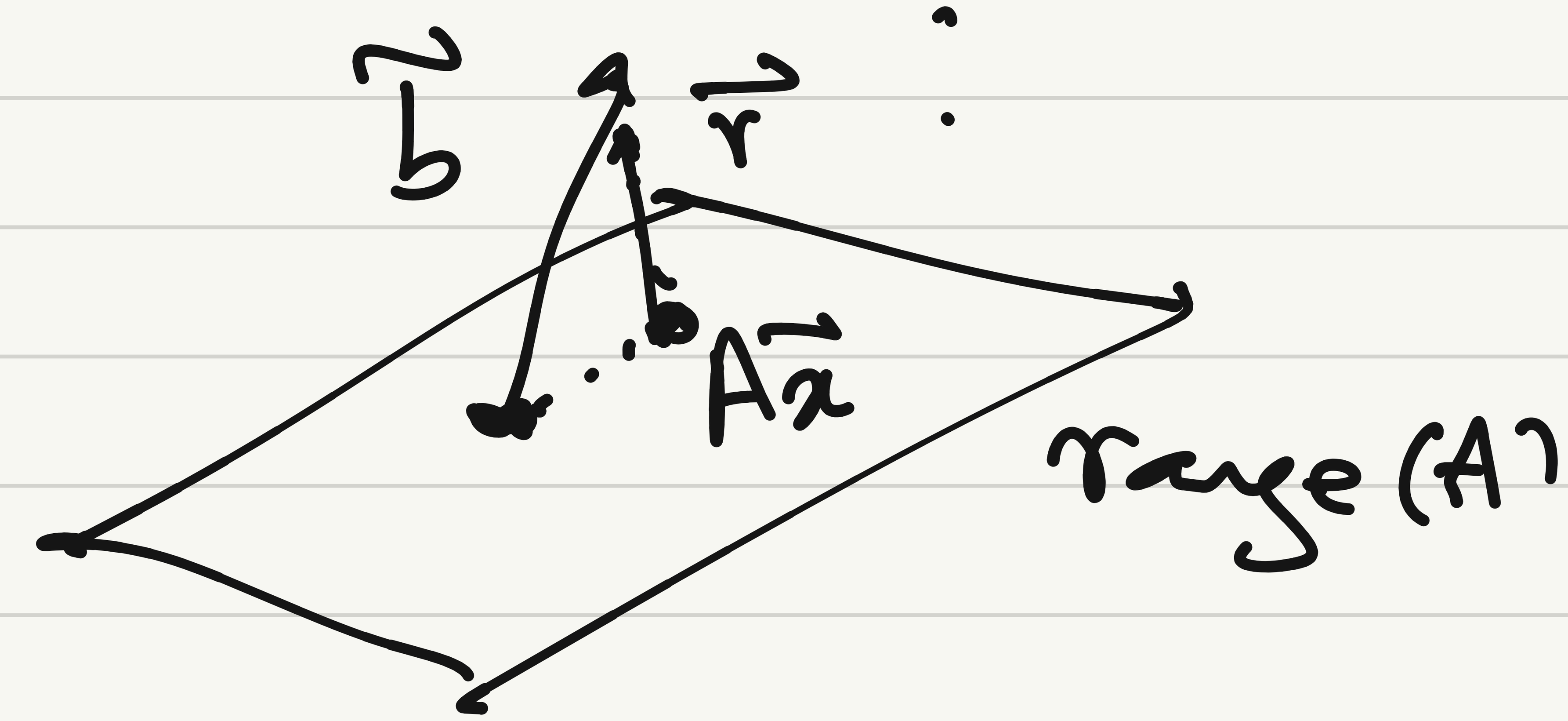
$a x_1^2 + b x_1 + c = y_1$

$a x_2^2 + b x_2 + c = y_2$

$a x_3^2 + b x_3 + c = y_3$

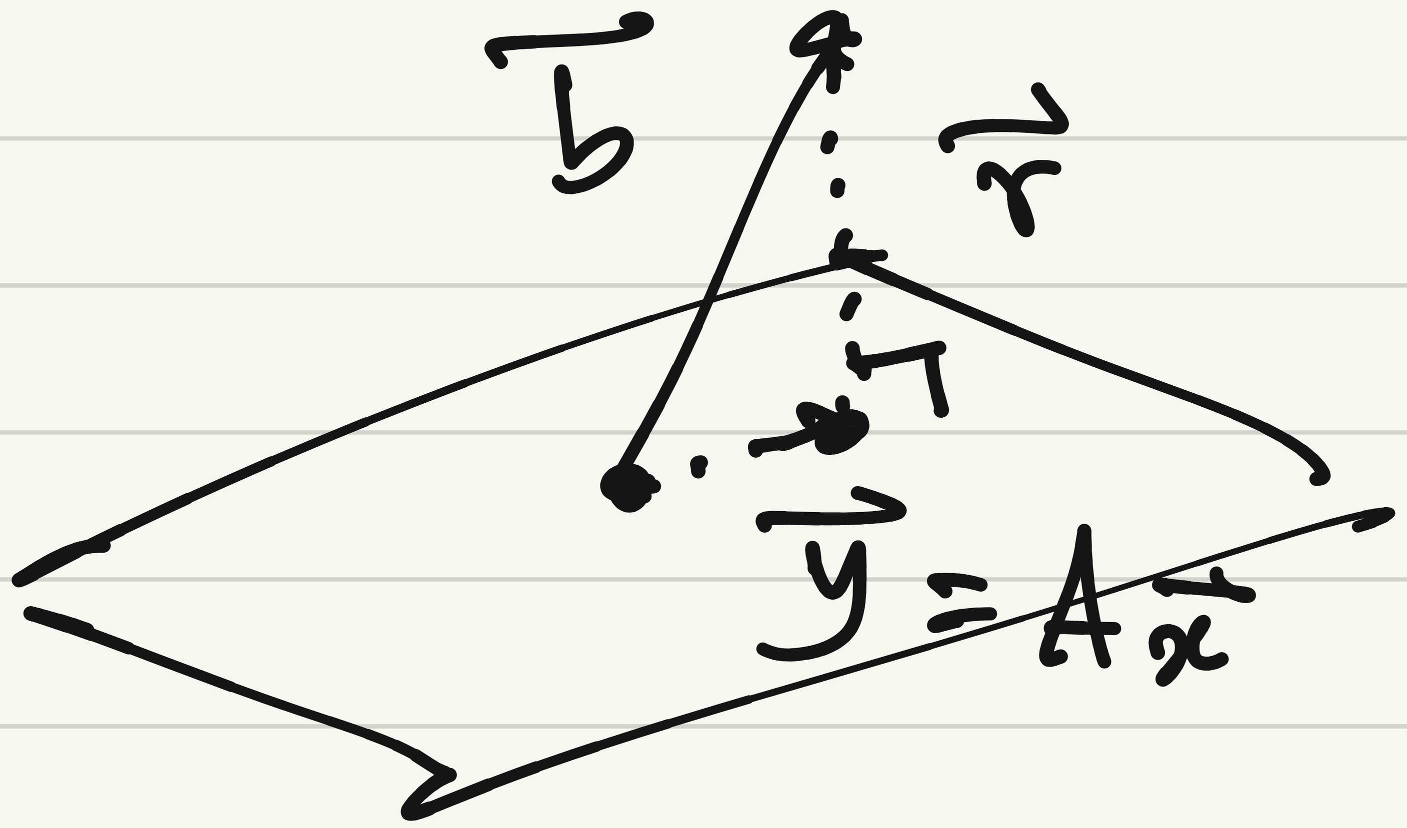
$\vdots$

$\underbrace{b - Ax} \rightarrow \boxed{\text{residual}}$ $\vec{r}$



$\min \; \|b - Ax\|_2$

$\min \sqrt{|b_1 - (Ax)_1|^2 + \cdots + |b_m - (Ax)_m|^2}$



If $\vec{x}$ minimizes $\|\vec{b} - Ax\|_2$

then $\vec{b} - A\vec{x} \perp \operatorname{range}(A)$

$$\vec{r} \perp \operatorname{range}(A) \iff \vec{r} \perp \vec{a}_j \iff \vec{a}_j^{\,*}\vec{r} = 0 \quad \forall j$$

$$\underbrace{\begin{bmatrix} - & \vec{a}_1^{\,*} & - \\ - & \vec{a}_2^{\,*} & - \\ & \vdots & \\ - & \vec{a}_n^{\,*} & - \end{bmatrix}}_{A^*} \vec{r} = 0 \Rightarrow \quad A^*(\vec{b} - A\vec{x}) = 0$$

$$\Rightarrow \quad \underbrace{A^*A}_{\mathbb{C}^{n\times n}}\vec{x} = \underbrace{A^*\vec{b}}_{\mathbb{C}^n}$$

$\boxed{\text{normal equations}}$

$$\vec{x} = \underbrace{(A^*A)^{-1}A^*}_{A^+} b$$

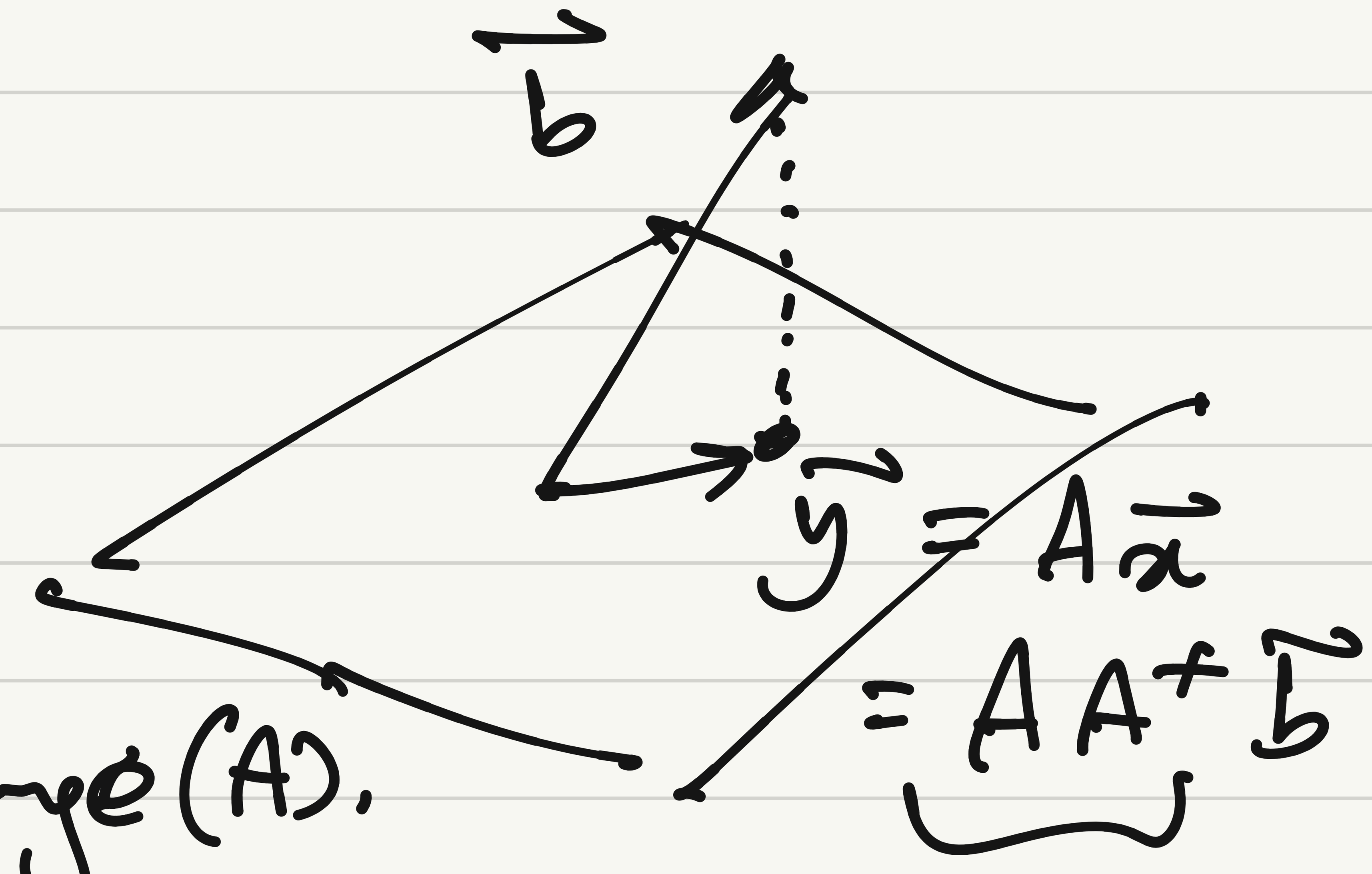
$$\vec{x} = A^+\vec{b}$$

$\boxed{\text{pseudoinverse}}$

$$\vec{x} = A^+\vec{b}$$

$$A^+ = (A^*A)^{-1}A^* \in \mathbb{C}^{n\times m}$$

$$A^+A = \underbrace{(A^*A)^{-1}}\,\underbrace{A^*A} = I$$



$\underbrace{AA^+}_{m\times m} \neq I$ $\qquad P = AA^+ =$ orthogonal projector onto range(A).

$\|\vec{b} - A\vec{x}\|_2 \Rightarrow \vec{x} = A^+ b$

$\vec{y} = A\vec{x} = P\vec{b}$

Algorithms for l. sq.

① Normal equations: compute A^*A, $A^*\vec{b}$

solve $\underbrace{(A^*A)}\vec{x} = A^*\vec{b} \longrightarrow \vec{x}$]

Cholesky factorization $\Rightarrow$ $\sim (m + \frac{n}{3})\, n^2$ flops

A^*A

$$A = \underbrace{\begin{bmatrix} \\ \\ \\ \end{bmatrix}}_{m \times n} \qquad \kappa(A) = \frac{\sigma_1}{\sigma_n}$$

$$\kappa(A^*A) = \frac{\sigma_1^2}{\sigma_n^2} = \kappa(A)^2$$

② QR factorization

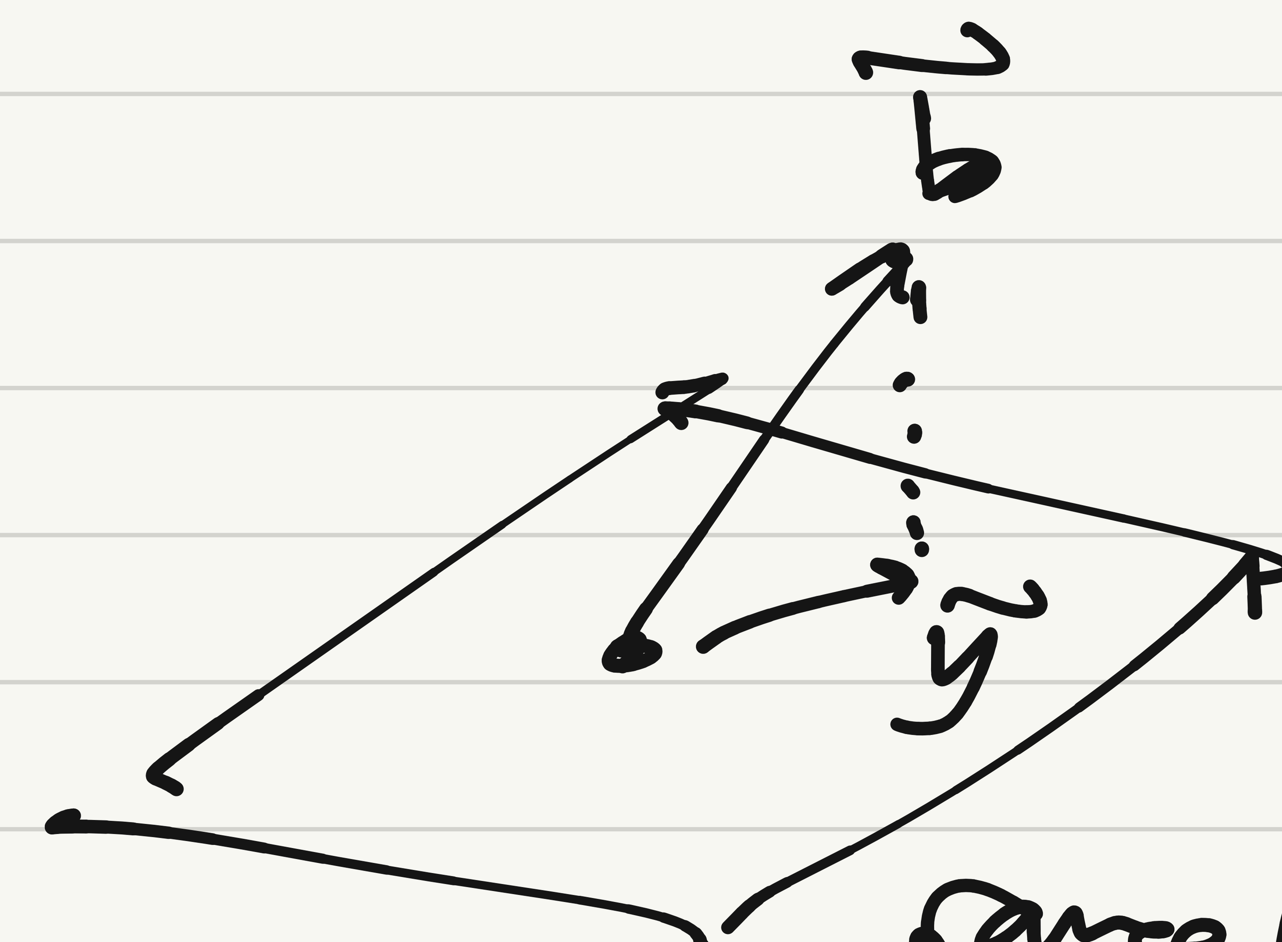
$A = \hat{Q}\hat{R}$

$\vec{y} = \hat{Q}\hat{Q}^*\vec{b}$

$\vec{y} = A\vec{x} = \hat{Q}\hat{R}\vec{x}$

$\Rightarrow \underbrace{R\vec{x} = \hat{Q}^*\vec{y}}$ Backward stable

$\sim (2m - \frac{2}{3}n)n^2$ flops



range(A)

= range($\hat{Q}$)

③ SVD $\quad A = \hat{U}\hat{\Sigma}V^*$

$\quad$ └ range$(\hat{U})$ = range(A)

$$\vec{y} = \hat{U}\hat{U}^*\vec{b}$$

$$\hat{U}\hat{\Sigma}V^*\vec{x} = \vec{y} \qquad \sim (2m + 11n)\,n^2 \text{ flops}$$

$$\hat{\Sigma}V^*\vec{x} = \underbrace{\hat{U}^* y}$$

<u>Conditioning of least-squares problems.</u>

$A \in \mathbb{C}^{m\times m}$

$A\vec{x} = \vec{b} \qquad$ inputs: $A, \vec{b}$, output: $\vec{x}$

$$\vec{x} = A^{-1}\vec{b} \qquad \kappa_{\vec{b}\to\vec{x}} = \limsup_{\|\delta b\|\to 0} \frac{\|\delta\vec{x}\|/\|\vec{x}\|}{\|\delta\vec{b}\|/\|\vec{b}\|} = \underbrace{\|A^{-1}\|\frac{\|\vec{b}\|}{\|\vec{x}\|}}$$

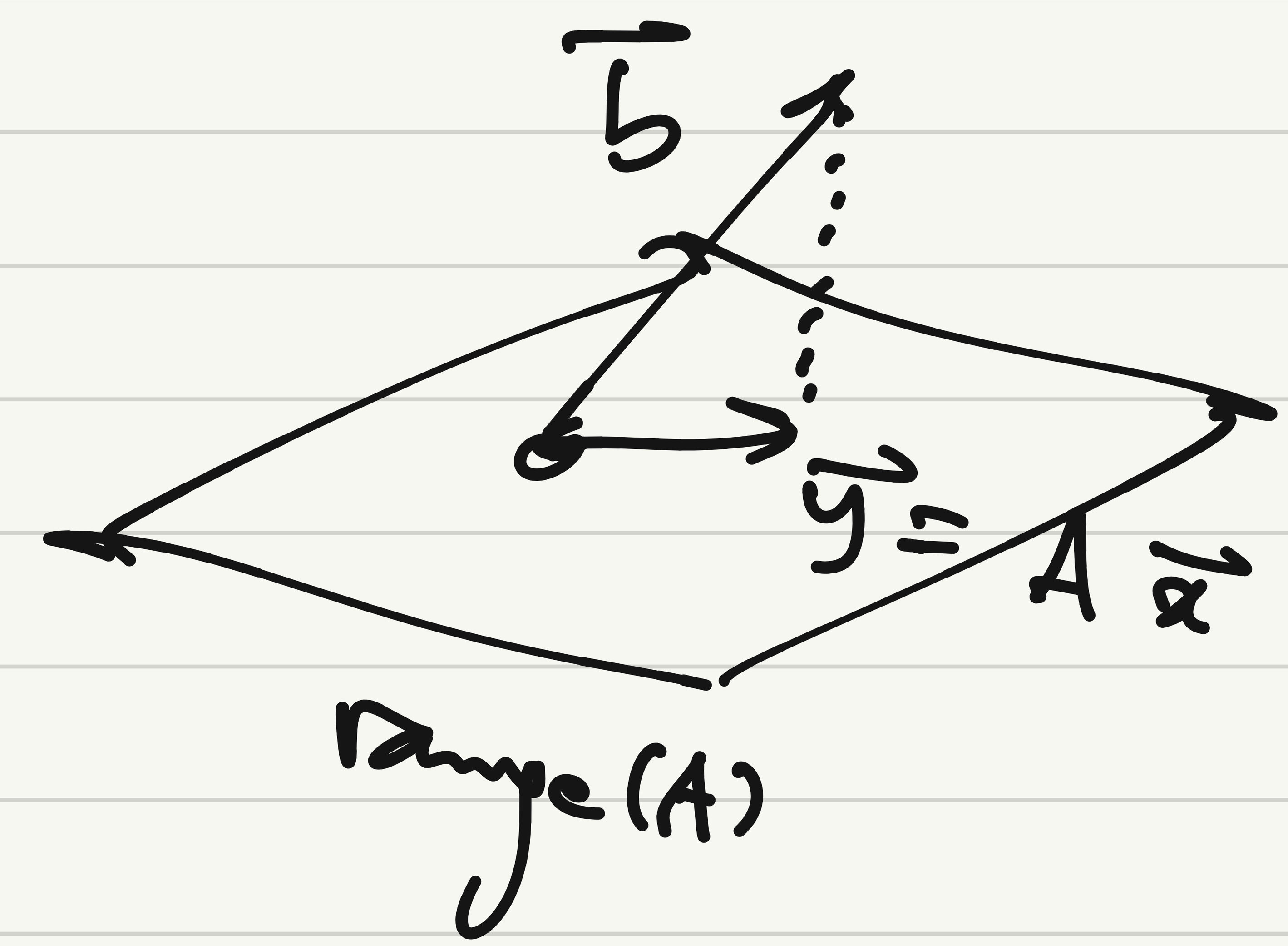
$$\kappa_{\vec{b}\to\vec{x}} = \frac{\|A^{-1}\|\,\|\vec{b}\|}{\|\vec{x}\|}$$

$$\frac{\|A\|\|\vec{x}\|}{\|\vec{b}\|} = \frac{\|A\|\cdot\|\vec{x}\|}{\underbrace{\|A\vec{x}\|}_{\vec{b}}} = \eta \in [1, \kappa(A)]$$

$$\frac{\|\vec{b}\|}{\|\vec{x}\|} = \frac{\|A\|}{\eta} \quad \Rightarrow \quad \kappa_{\vec{b}\to\vec{x}} = \frac{\|A^{-1}\|\,\|A\|}{\eta} = \frac{\kappa(A)}{\eta}$$

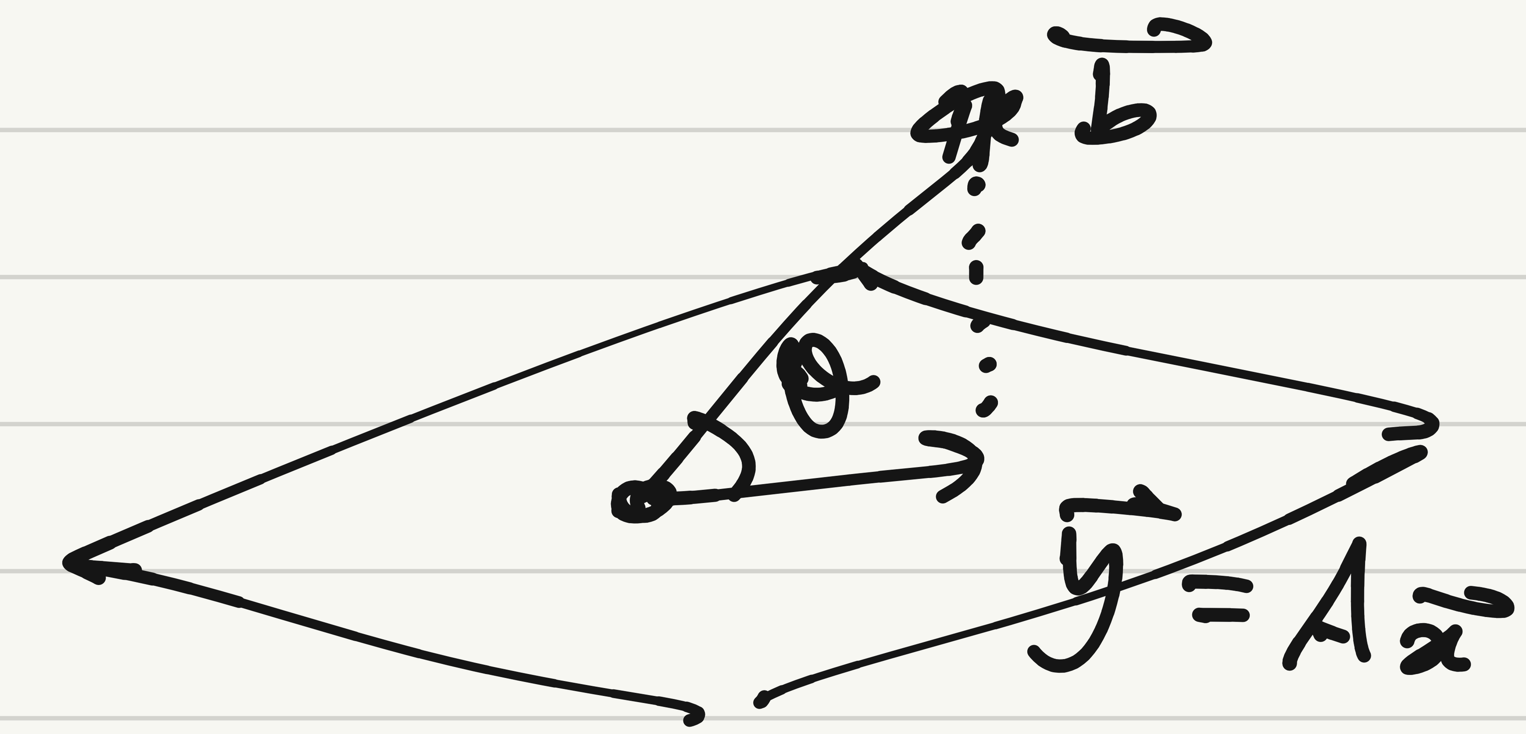
$$\kappa_{A\to\vec{x}} = \kappa(A)$$

$$\min \|\underset{\uparrow}{\vec{b}} - \underset{\uparrow}{A}\vec{x}\| \longrightarrow \vec{y}, \vec{x}$$



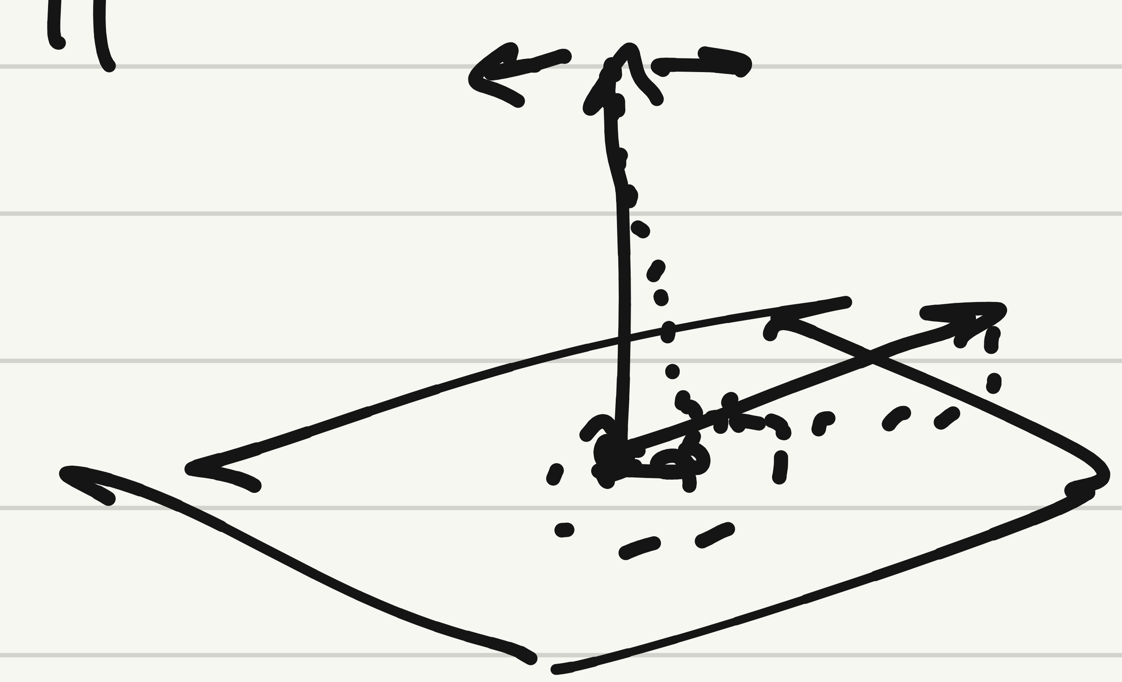
$\kappa_{\vec b \to \vec y}$ $\qquad \vec y = P\vec b$

$$\|\delta \vec y\| \le \|\delta \vec b\|$$



$$= \frac{\|\delta\vec y\|/\|\vec y\|}{\|\delta \vec b\|/\|\vec b\|} = \frac{\|\vec b\|}{\|\vec y\|} = \frac{1}{\cos\theta}$$

$$\cos\theta = \frac{\|\vec y\|}{\|\vec b\|}$$



$\kappa_{\vec b \to \vec x} = ?$

$$\hat Q \hat R \vec x = \vec y \to \hat R \vec x = \hat Q^* \vec y$$

$$\eta = \frac{\|A\|\,\|x\|}{\|y\|}$$

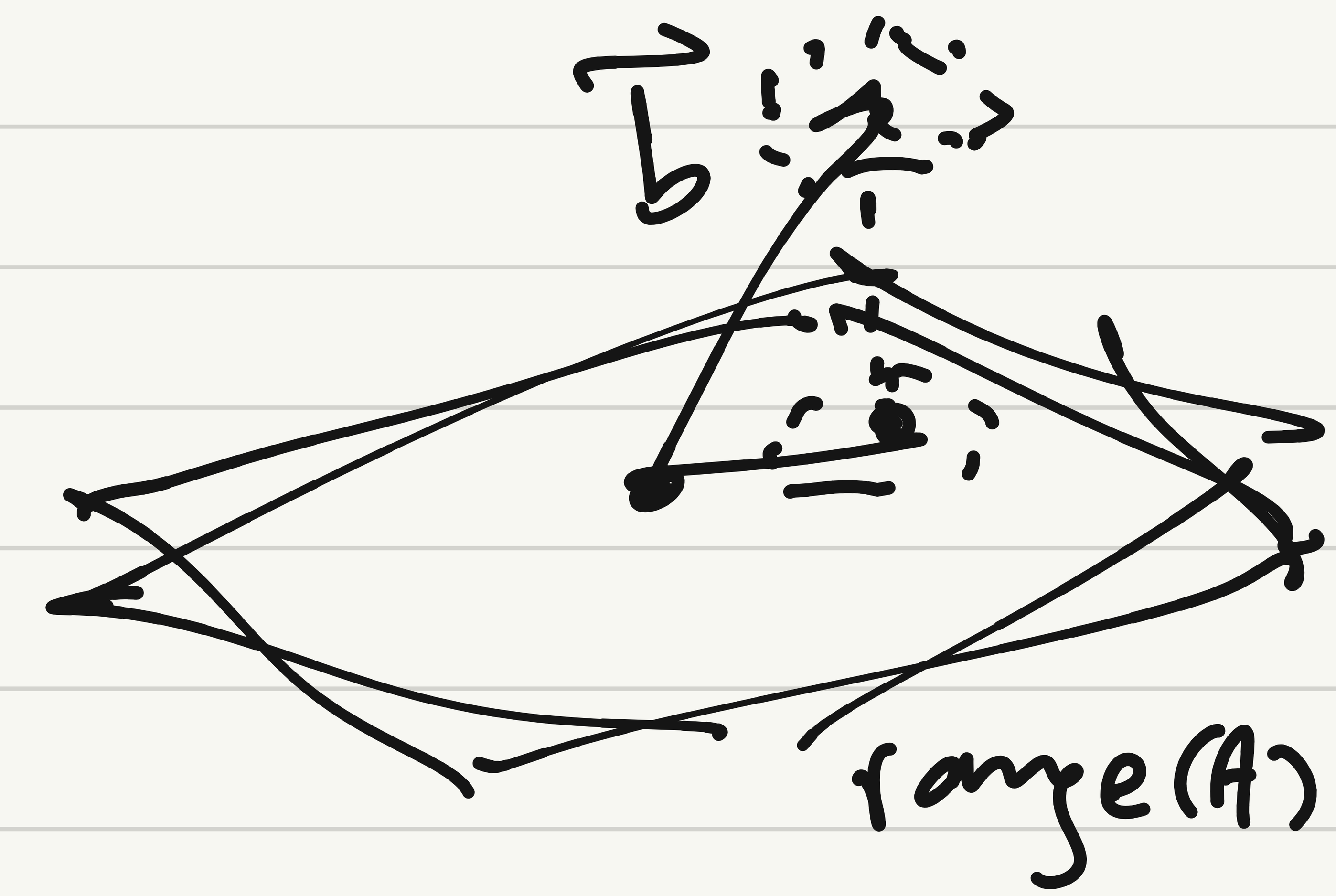
$\hat R$ has same singular values as A

$\hat R^{-1}$ " " " " " A^+ : $\frac{1}{\sigma_n}, \dots, \frac{1}{\sigma_1}$

$$\kappa_{\vec y \to \vec x} = \frac{\|\hat R^{-1}\|\,\|\vec y\|}{\|\vec x\|} = \|\hat R^{-1}\| \cdot \frac{\|A\|}{\eta} = \kappa(A)/\eta$$

$$\kappa_{\vec{b}\to\vec{y}} = \boxed{\frac{1}{\cos\theta}}$$

$$\kappa_{\vec{y}\to\vec{x}} = \frac{\kappa(A)}{\eta} \implies \kappa_{\vec{b}\to\vec{x}} = \boxed{\frac{\kappa(A)}{\eta\cos\theta}}$$



$$\kappa_{A\to\vec{y}} \le \boxed{\frac{\kappa(A)}{\cos\theta}}$$

$$\kappa_{A\to\vec{x}} \le \boxed{\underline{\kappa(A)} + \frac{\kappa(A)^2\tan\theta}{\eta}}$$

normal eqs. $\underline{\kappa(A)^2}$

Cond. nums. are large if:

1. $\kappa(A)$ is large
2. $\cos\theta \approx 0 \iff \vec{b}$ is nearly ortho. to range(A)]
3. $\eta \approx 1 \iff \|\vec{y}\|$ is close to $\|A\|\,\|\vec{x}\|$