Theorem: $A \in \mathbb{R}^{n\times n}$ regular, $b \in \mathbb{R}^n$, $Ax=b$, $A(x+\delta x) = b+\delta b$

$$\Longrightarrow \frac{\|\delta x\|}{\|x\|} \leq \kappa(A) \frac{\|\delta b\|}{\|b\|}$$

Proof: $b = Ax$, $\delta x = A^{-1}(b+\delta b) - x = A^{-1}\delta b$

$$\|b\| = \|Ax\| \leq \|A\|\,\|x\| , \quad \|\delta x\| \leq \|A^{-1}\|\,\|\delta b\|$$

$$\xrightarrow{\text{multiply}} \|b\|\,\|\delta x\| \leq \underbrace{\|A\|\,\|A^{-1}\|}_{\kappa(A)} \|x\|\,\|\delta b\|$$

$$\Longrightarrow \frac{\|\delta x\|}{\|x\|} \leq \kappa(A) \frac{\|\delta b\|}{\|b\|} \qquad \square.$$

Example: $A = \begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{3} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} \\ \frac{1}{3} & \frac{1}{4} & \frac{1}{5} \end{pmatrix} \in \mathbb{R}^{3\times 3}$, invertible,

$\kappa_2(A) \cong 524$

We solve $Ax = b$ with $b = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$ and b are measurements with potential error of 10^{-4}, i.e.

$$\underbrace{b + \delta b = \begin{pmatrix} 1 \\ \varepsilon \\ 0 \end{pmatrix}, \ |\varepsilon| \leq 10^{-4}}_{\text{error of } 0.01\%}$$

Then x satisfies $\|x\|_2 \sim 48$, $x = \begin{pmatrix} 9 \\ -36 \\ 30 \end{pmatrix}$

$$\frac{\|\delta x\|_2}{48} \leq 524 \cdot \frac{10^{-4}}{1}$$

$\longrightarrow \|\delta x\|_2 \lesssim 2.5 \longrightarrow$ error in x of $\approx 5\%$

$\longrightarrow$ relative error potentially increases by a factor of ~ 500, i.e. by the condition number.

§2.7 Least squares problems

Consider an overdetermined system

$$\begin{pmatrix} 3 & 1 \\ 1 & 1 \\ 4 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 2 \end{pmatrix}, \quad A \in \mathbb{R}^{m \times n}, \quad b \in \mathbb{R}^m, \quad m \geq n$$

This system does, in general, not have a solution, but we can try to find $x \in \mathbb{R}^2$ such that $Ax - b \approx 0$.
This can be formulated as least squares problem

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

which is equivalent with

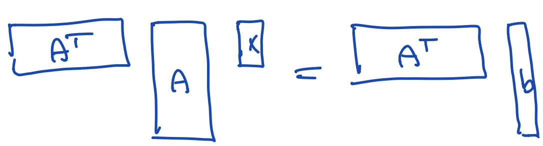
$$\min_{x \in \mathbb{R}^n} \|Ax - b\|_2^2 \leftarrow \text{"least squares"}$$

Since for any vector $y \in \mathbb{R}^m$: $\|y\|_2^2 = y^T y$, we can write

$$\|Ax - b\|_2^2 = (Ax-b)^T (Ax-b) = \underbrace{x^T A^T A x - \overbrace{(x^T A^T b + b^T A x)}^{2x^T A^T b} + b^T b}_{\text{quadratic form in } x.}$$

Minimum is characterized by

$$A^T A x = A^T b \quad \text{normal equations}$$



One should avoid computation of A^TA as this can be expensive if m, n are large, and A^TA can be poorly conditioned.

For instance: $A = \begin{pmatrix} \varepsilon & 0 \\ 0 & 1 \end{pmatrix}$, $B = A^TA$

$$\kappa_2(A) = \|A\|_2 \|A^{-1}\|_2 = 1 \cdot \varepsilon^{-1} = \frac{1}{\varepsilon}$$

$$\kappa_2(B) = \|A^TA\|_2 \|(A^TA)^{-1}\|_2 = \frac{1}{\varepsilon^2}$$

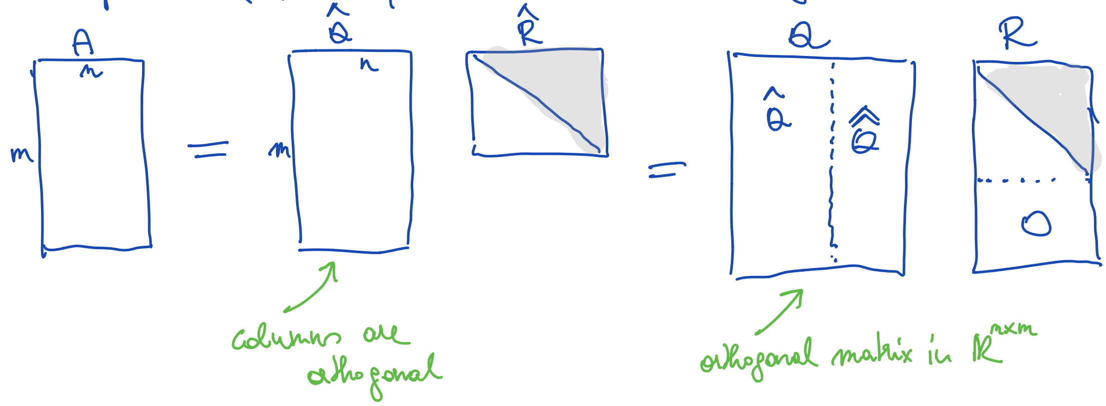
ε is very small, $\kappa_2(A) = \frac{1}{\varepsilon} \ll \kappa_2(A^TA) = \frac{1}{\varepsilon^2}$

Theorem: Let $A \in \mathbb{R}^{m \times n}$, $m \geq n$. Then

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

where $\hat{R}$ is upper triangular matrix, $\hat{R} \in \mathbb{R}^{n \times n}$, $\hat{Q} \in \mathbb{R}^{m \times n}$ with $\hat{Q}^T\hat{Q} = I_{n \times n}$.

If $\mathrm{rank}(A) = n$, then $\hat{R}$ is non-singular.



Theorem: QR-factorization for least squares solve

$$\min_{x \in \mathbb{R}^n} \|Ax - b\|_2^2.$$ The solution x can be

computed as solution of $\underbrace{\hat{R}x = \hat{Q}^T b}_{\text{requires one backward subst.}}$.

Proof: $\|Ax-b\|_2^2 = (Ax-b)^T(Ax-b)$

$= (Ax-b)^T \underbrace{Q\,Q^T}_{I}(Ax-b)$ $A = QR = \hat{Q}\hat{R}$

$R = Q^T A$

$= \|Q^T(Ax-b)\|_2^2 = \|Rx - Q^T b\|_2^2$

$= \left\| \begin{pmatrix} \hat{R}x \\ 0 \end{pmatrix} - \begin{pmatrix} \hat{Q}^T b \\ b_2 \end{pmatrix} \right\|_2^2 = \|\hat{R}x - \hat{Q}^T b\|_2^2 +$

$+ \|b_2\|_2^2 \geq \|b_2\|_2^2$, $b_2 := \hat{\hat{Q}}^T b$

$\longrightarrow$ The quantity $\|Ax-b\|_2^2$ can be made smallest possible by making $\|\hat{R}x - \hat{Q}^T b\|_2 = 0$, i.e. $\hat{R}x = \hat{Q}^T b$.

Thus, by solving $\hat{R}x = \hat{Q}^T b$, we find the solution to the least squares problem. $\square$.