- Exam 1 results: not yet
- Quiz deadlines
- Class fb

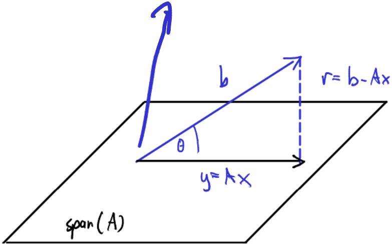
$A\vec{x} \longrightarrow \vec{b}$

normal eq: $A^T A \vec{x} = A^T \vec{b}$

Goals: ↳ why not?

- Cond LSQ
- $QR = A$
- Householder refl.

# Sensitivity and Conditioning of Least Squares




Relate $\|A\boldsymbol{x}\|_2$ and $\|\boldsymbol{b}\|_2$ with $\theta$ via trig functions.

$$\cos\theta = \frac{\|Ax\|_2}{\|b\|_2}$$

# Sensitivity and Conditioning of Least Squares (II)

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

$$\frac{\|\Delta x\|}{\|x\|} \le \kappa(A) \frac{\|\Delta b\|}{\|b\|}$$

Derive a conditioning bound for the least squares problem.

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

$$\frac{\|\Delta x\|_2}{\|x\|_2} = \frac{\|A^+\Delta b\|}{\|x\|_2} \le \|A^+\|_2 \frac{\|\Delta b\|}{\|x\|}$$

$$= \frac{\kappa_2(A)}{\cancel{\|A^+\|_2}} \cancel{\|A^+\|_2} \frac{\|b\|_2}{\|A\|_2 \|x\|_2} \frac{\|\Delta b\|_2}{\|b\|_2}$$

To-do →

$$\le \kappa_2(A) \underbrace{\frac{\|b\|_2}{\|Ax\|_2}}_{1/\cos\theta} \frac{\|\Delta b\|_2}{\|b\|_2}$$

cond. of solve for x from proj.

→ proj. to plane

What values of $\theta$ are bad?

$$\vec{b} \perp \text{colspan}(A\vec{x})$$

$\kappa_2(A) = \|A\|\,\|A^{-1}\|$ if square & inv.

$\kappa_2(A) = \infty$ if square & not inv.

$\kappa_2(A) = \sigma_1/\sigma_n = \|A\|\,\|A^+\|$ if T & s & ~~inv.~~ full rank

$\kappa_2(A) = \infty$ & ~~not inv.~~ not full rank

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

$\Leftrightarrow U \Sigma V^T \vec{x} = \vec{b}$

$\Leftrightarrow \Sigma \vec{y} = U^T \vec{b}$ $\quad \vec{y} = V^T \vec{x}$

$\Sigma \to \begin{bmatrix} \sigma & & 0 \\ & \ddots & \sigma \\ & 0 & \end{bmatrix}$

$\vec{b} \in \operatorname{colspan}(A)$ $\Leftrightarrow$ "bottom part of $U^T b$ is zero"

$$\begin{bmatrix} 2 & \\ & 1 \\ & \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \overset{?}{=} \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

$$0 \cdot x_1 + 0 \cdot x_2 = 3$$

cond of solving

$$\Sigma_{top}\, \vec{y} = U^T \vec{b}$$

$$\begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{bmatrix} \; ?$$

$$\sigma_1 / \sigma_n = \|A\|_2 \, \|A^+\|_2$$

exercise for the reader

top-half: "the solvable bit" of $A\vec{x} \cong \vec{b}$

$A\vec{x} \approx \vec{b} \iff$ Find $\vec{x}$ so that

$$\|A\vec{x} - \vec{b}\|_2 \to \min!$$

$$\min_{\vec{x}} \|Ax - b\|_2 = \min_x \|U \Sigma V^T \vec{x} - \vec{b}\|_2$$

$$= \min \|U^T (U \Sigma V^T \vec{x} - \vec{b})\|_2$$

$$= \min_x \|\Sigma V^T \vec{x} - U^T b\|_2$$

$$(y = V^T x) \to \min_y \|\Sigma \vec{y} - \underbrace{U^T b}_{U^T b}\|_2$$

$$\min_y \left\| \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \\ & 0 & \end{pmatrix} \vec{y} - \begin{bmatrix} \vdots \end{bmatrix} \right\|_2$$

find $\vec{y} = \Sigma_{top}^{-1} U^T \vec{b}$

$$\vec{x} = V \Sigma_{top}^{-1} U^T \vec{b}$$

# Sensitivity and Conditioning of Least Squares (III)

Any comments regarding dependencies?

unlike solve, depends on $\kappa(A)$ and $\vec{b}$

What about changes in the matrix?

$$\frac{\|\Delta x\|}{\|x\|} \leq \left[\operatorname{cond}(A)^2 \tan\theta + \operatorname{cond}(A)\right] \frac{\|\Delta A\|}{\|A\|}$$

deps on $\vec{b}$

two cases: $\tan(\theta)$ small or not.

# Transforming Least Squares to Upper Triangular

Suppose we have $A = QR$, with $Q$ square and orthogonal, and $R$ upper triangular. This is called a QR factorization.

How do we transform the least squares problem $A\boldsymbol{x} \cong \boldsymbol{b}$ to one with an upper triangular matrix?

$$\min_{x} \|Ax - b\|_2$$

$$= \min_{\vec{x}} \|QR\vec{x} - \vec{b}\|_2$$

$$= \min_{x} \|Q^T(QR\vec{x} - b)\|_2 = \min_{x} \|R\vec{x} - Q^T b\|_2$$

$$\begin{pmatrix} \diagdown & \\ 0 & \end{pmatrix} \vec{x} = [\ ] \leftarrow Q^T b$$

# Simpler Problems: Triangular

What do we win from transforming a least-squares system to upper triangular form?

$\tilde{x} = \begin{bmatrix} \tilde{x}_1 \\ x_2 \end{bmatrix}$ $\quad \|x\|_2^2 = \|x_1\|^2 + \|x_2\|^2$

How would we minimize the residual norm?

$$\|\tilde{r}\|_2^2 = \|Ax - b\|_2^2 = \|(Q^T b)_{top} - R_{top}\tilde{x}\|^2$$

$$+ \|(Q^T b)_{bottom}\|_2^2$$

$$\text{set } \tilde{x} = R_{top}^{-1}(Q^T b)_{top} \Rightarrow \|(Q^T b)_{top} - R_{top}\tilde{x}\|^2 = 0$$

# Computing QR

- Gram-Schmidt
- Householder Reflectors
- Givens Rotations

✓**Demo:** Gram-Schmidt–The Movie [cleared] (shows *modified G-S*)
**Demo:** Gram-Schmidt and Modified Gram-Schmidt [cleared]
✓**Demo:** Keeping track of coefficients in Gram-Schmidt [cleared]
Seen: Even modified Gram-Schmidt still unsatisfactory in finite precision arithmetic because of roundoff.

NOTE: Textbook makes further modification to 'modified' Gram-Schmidt:

- Orthogonalize *subsequent* rather than *preceding* vectors.
- Numerically: no difference, but sometimes algorithmically helpful.

# Economical/Reduced QR

Is QR with square $Q$ for $A \in \mathbb{R}^{m \times n}$ with $m > n$ efficient?