Last time: SVD of matrix $A \in \mathbb{C}^{m \times n}$

$$A = \underset{\uparrow}{U} \; \underset{\uparrow}{\Sigma} \; V^*$$

$U \in \mathbb{C}^{m \times m}$, $U^* U = I_m$

$\Sigma \in \mathbb{R}^{m \times n}_{\geq 0}$, $\Sigma = \operatorname{diag}(\sigma_1, \cdots, \sigma_p)$, $p = \min\{m, n\}$

$V \in \mathbb{C}^{n \times n}$, $V^* V = I_n$

- Existence: ① $A^* A = V \underbrace{\begin{bmatrix} \sigma_1^2 & & \\ & \ddots & \\ & & \sigma_n^2 \end{bmatrix}}_{\Sigma^2} V^*$

  ② $U \Sigma = A V$

- Practical algorithm: Solve eigenvalue problem for

$$H = \begin{bmatrix} 0 & A^* \\ A & 0 \end{bmatrix} \leftarrow \text{Hermitian}$$

use Golub-Kahan bidiagonalization: operation count $\approx 4mn^2$ FLOPs
(will go into detail when we talk about eigenvalue problems)

- Application 1: Point cloud registration
- Application 2: Overdetermined least-squares

Given $b(a) \in L^2([0,1])$

Find n-degree polynomial $p(a) \in P_n([0,1])$

such that $\min_{p \in P_n} \int_0^1 |p(a) - b(a)|^2 \, da$

Discretize the problem:

quadrature: $\int_0^1 f(a) \, da \approx \frac{1}{m} \sum_{i=1}^{m} f(a_i)$, $a_i = \frac{i-1}{m-1}$, $i = 1, \cdots, m$

$$p(x) = \sum_{k=0}^{n-1} x_k a^k$$

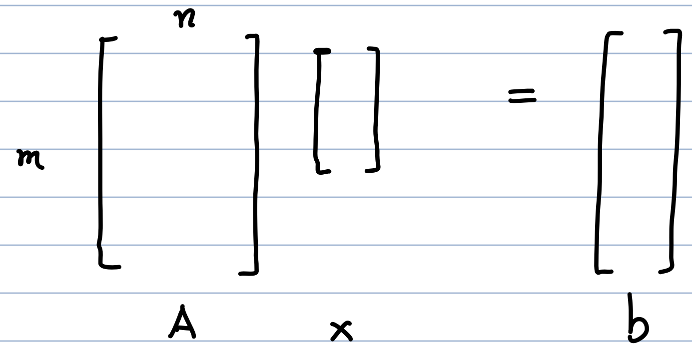
$$\Rightarrow \quad \min_{c \in \mathbb{R}^n} \frac{1}{m} \sum_{i=1}^{m} \left| \sum_{k=0}^{n-1} x_k a_i^k - b(x_i) \right|^2$$

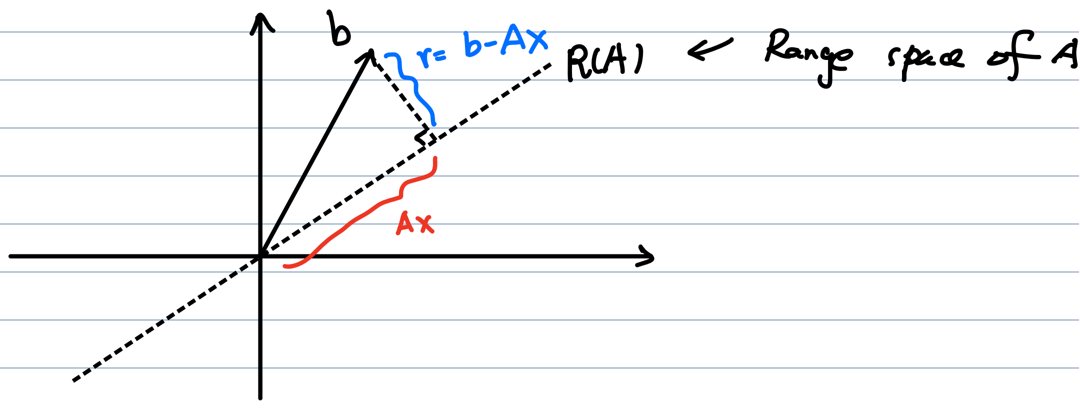
Let $A = \begin{bmatrix} 1 & a_1 & \cdots & a_1^{n-1} \\ 1 & a_2 & \cdots & a_2^{n-1} \\ \vdots & \vdots & & \vdots \\ 1 & a_m & \cdots & a_m^{n-1} \end{bmatrix}$, $\quad b = (b(x_1), \cdots, b(x_m))^T$

$x = (x_1, \cdots, x_n)^T$

$$\Rightarrow \quad \min_x \|Ax - b\|_2^2 \quad \leftarrow \text{Least-squares problem}$$

m equations $>$ n variables





- Solve least-squares via normal equations

$$\hat{x} \in \arg\min_x \|Ax - b\|_2^2$$

$$\Leftrightarrow \quad r = b - A\hat{x} \perp R(A)$$

$$\Leftrightarrow \quad b - A\hat{x} \in \mathcal{N}(A^*)$$

$$\Leftrightarrow \quad A^*A\hat{x} = A^*b \quad \leftarrow \text{Normal equations}$$

assume $\operatorname{rank}(A) = n$ so $\operatorname{rank}(A^*A) = \operatorname{rank}(A) = n$

and A^*A invertible

- Solving least-squares via normal equations

Step 1: compute $C = A^*A$, $d = A^*b$

Step 2: Solve $C\hat{x} = d$ operation count $\approx 2mn^2$ FLOPs $(m \gg 1)$

- Solving normal equations directly can suffer from ill-conditioning

For the least square problem using monomials,

as $m \to +\infty$, $\frac{1}{m}(A^*A)_{ij} = \frac{1}{m}\sum_{k=1}^{m} a_k^{i+j-2}$

$$= \frac{1}{m}\sum_{k=1}^{m}\left(\frac{k-1}{m-1}\right)^{i+j-2}$$

$$\to \int_0^1 a^{i+j-2}\,da = \frac{1}{i+j-1}$$

So $\frac{1}{m}A^*A \to H_n$ Hilbert matrix — ill-conditioned !

Beyond NLA: monomials are "bad" basis, choose basis that are orthogonal to each other

In general, $\kappa_2(A^*A) = \frac{\sigma_1^2}{\sigma_n^2} \gg \sigma_1/\sigma_n \; (= \kappa_2(A))$

Forward error $\approx \kappa_2^2(A)\,\varepsilon$

backward error

- Solve least-squares via SVD

Let $A = U\Sigma V^*$

$$\min_x \| U\Sigma V^* x - b\|_2^2$$

Let $d = U^*b$, $y = V^*x$

$$\min_y \|\Sigma y - d\|_2^2 = \min_{y\in\mathbb{C}^n} \left\| \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \\ & 0 & \end{bmatrix}\begin{bmatrix} y_1 \\ \vdots \\ y_n\end{bmatrix} - \begin{bmatrix} d_1 \\ \vdots \\ d_m\end{bmatrix}\right\|^2$$

Let $\Sigma^+ = \begin{bmatrix} d_1/\sigma_1 & & & \\ & \ddots & & \\ & & d_n/\sigma_n & 0 \end{bmatrix}$

$$\hat{y} := \Sigma^+ d = \operatorname{argmin} \|\Sigma y - d\|_2^2$$

hence $\hat{x} = V\hat{y} = \underbrace{V\Sigma^+ U^*}_{A^+} b \in \operatorname{argmin} \|Ax - b\|^2$

A^+ pseudoinverse of A

Actually, from normal equation,

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

$$= (V\Sigma^*\Sigma V^*)^{-1} V\Sigma^* U^* b$$

$$= V(\Sigma^*\Sigma)^{-1} V^* V \Sigma^* U^* b$$

$$= V\Sigma^+ U^* b$$

Algorithm:

Step 1: Compute SVD : $A = U\Sigma V^*$

operation count $\approx 4mn^2$ FLOPs

Step 2: $\hat{x} = V\Sigma^+ U^* b$

- Stability of least-squares

Define $\kappa_2(A) = \|A\|_2 \|A^+\|_2 = \sqrt{\kappa_2(A^*A)}$

Thm (Wedin) Let $A \in \mathbb{R}^{m\times n}$, $A + \Delta A$ both be of full rank

Let $\|b - Ax\|_2 = \min$. $r = b - Ax$

$\|(b+\Delta b) - (A+\Delta A)y\|_2 = \min$, $s = b + \Delta b - (A+\Delta A)y$

$\|\Delta A\|_2 / \|A\|_2$, $\|\Delta b\|_2 / \|b\|_2 \leq \varepsilon$

Then provided that $\kappa_2(A)\varepsilon < 1$

we have

$$\frac{\|x-y\|_2}{\|x\|_2} \leq \frac{\kappa_2(A)\,\varepsilon}{1-\kappa_2(A)\,\varepsilon}\left(2+(\kappa_2(A)+1)\frac{\|r\|_2}{\|A\|_2\|x\|_2}\right)$$

$\approx \kappa_2(A)\,\varepsilon$ when $\|r\|_2$ small

$\approx \kappa_2^2(A)\,\varepsilon$ otherwise

$$\frac{\|r-s\|_2}{\|b\|_2} \leq (1+2\kappa_2(A))\,\varepsilon_{mach}$$

These bounds are approximately attainable

Pf: See Higham Thm 20.1 ☒

Remark: The first bound is usually interpreted as saying that the sensitivity of least-squares is measured by $\kappa_2(A)$ when $\|r\|$ is small or zero and by $\kappa_2^2(A)$ otherwise

<u>Thm</u> Solving least-squares via SVD is backward stable. The computed $\hat{x}$ satisfies

$$\hat{x} = \arg\min_x \|(A+\Delta A)x + b + \Delta b\|_2$$

and $\|\Delta A\|/\|A\| \cdot \|\Delta b\|/\|b\| \leq C_{mn}\,\varepsilon_{mach}$

Summary:

method	normal eqn	SVD
conditioning	$\approx \kappa_2^2(A)$	$\approx \kappa_2(A)$ ($\|r\|$ small)
operation count	$\approx 2mn^2$ FLOPs	$\approx 4mn^2$ FLOPs

- Solving least-squares via QR factorization

Computing SVD is expensive. can we work with orthogonal transform but lower cost?

• (reduced) QR factorization

$$A = Q \quad R$$

$R \in \mathbb{C}^{n\times n}$
upper triangular matrix

Not $QQ^* = I_m$

$Q \in \mathbb{C}^{m\times n}$
$Q^*Q = I_n$
orthonormal columns $\quad (m \geq n)$

when $\operatorname{rank}(A) = n$, $\Rightarrow \operatorname{rank}(R) = n$

hence $R(A) = R(Q)$

Let $Q = [q_1 \cdots q_n]$, $\quad q_i \in \mathbb{C}^m$

projection onto $R(A)$

Then $\quad P_A x = P_Q x = \sum_{i=1}^{n} q_i (q_i^* x) = QQ^* x$

Hence $\quad \hat{x} \in \arg\min_x \|Ax-b\|_2^2$

$\iff \quad r = b - A\hat{x} \perp R(A)$

$\iff \quad P_Q r = 0$

$\iff \quad QR\hat{x} = QQ^*b$

$\iff \quad R\hat{x} = Q^*b$

$\iff \quad \hat{x} = R^{-1}Q^*b$

Actually, from normal equations,

$$\hat{x} = (A^*A)^{-1}A^*b = (R^*R)^{-1}R^*Q^*b = R^{-1}Q^*b$$