5, Least Squares

goal: $A \in \mathbb{R}^{m \times n}$, $m \neq n$, solve $A\vec{x} = \vec{b}$

<u>Def (Least squares solution)</u> $\vec{x}$ solves $A\vec{x} = \vec{b}$ st.

$$\|b - Ax\|_2 = \min_y \{ \|b - Ay\|_2 , \ y \in \mathbb{R}^n \}$$

<u>Normal equations</u> $\vec{x}$ solves $A^T A \vec{x} = A^T \vec{b}$

$\Leftrightarrow$ $\vec{x}$ solves $\|b - Ax\|_2 = \min_{y \in \mathbb{R}^n} \|b - Ay\|$

Proof: $\pi = \pi(t) : \mathbb{R} \to \mathbb{R}$

$t \mapsto \|\vec{b} - A(\vec{x} + t\vec{v})\|_2^2$ with $\vec{y} := \vec{x} + t\vec{v}$

$$\Rightarrow \pi(t) = \langle b - A(x+tv), b - A(x+tv) \rangle = \langle b - Ax, b - Ax - Atv \rangle + \langle -Atv, b - Ax - Atv \rangle$$

$$= \langle b - Ax, b - Ax \rangle + \langle b - Ax, -Atv \rangle + \langle -Atv, b - Ax \rangle + \langle -Atv, -Atv \rangle$$

$$= \langle b - Ax, b - Ax \rangle - 2t \langle b - Ax, Av \rangle + t^2 \|Av\|^2$$

minimum of π is at $t = 0$:

$$0 \overset{!}{=} \pi'(0) = +2 \langle b - Ax, Av \rangle = 2v^T A^T (b - Ax) \xRightarrow{v \text{ arbitrary}} A^T A x = A^T b \ \blacksquare$$

(also works in reverse)

<u>QR solution of least squares</u> $A \in \mathbb{R}^{m \times n}$, $A = QR$, $Q \in \mathbb{R}^{m \times n}$, $R \in \mathbb{R}^{m \times n}$

$\vec{x}$ solves least squ. by finding $R^* \vec{x} = b^*$

with R^* is the square, upper triang. part of $R = \begin{pmatrix} R^* \\ 0 \end{pmatrix}$

and $\vec{b}^* = (Q^T \vec{b})_{i = 1, \dots n}$ (neglecting $i = n+1, \dots m$)

Q is length-preserving

Proof: minimize $\|Ay - b\|_2^2 = \|QRy - b\|^2 = \|Q(Ry - Q^T b)\|^2 = \|Ry - Q^T b\|^2$

$$= \left\| \begin{pmatrix} R^* \\ 0 \end{pmatrix} y - \begin{pmatrix} b^* \\ \tilde{b}_{rest} \end{pmatrix} \right\|^2 = \|R^* y - b^*\|^2 + \|\tilde{b}_{rest}\|$$

$$\Rightarrow x = y = R^{*-1} \vec{b}^* \quad \blacksquare$$

<u>Underdetermined systems</u> if $m < n \Rightarrow$ sol to $Ax = b$

not unique. look for minimum norm solution: find x st.

$$\|x\|_2 = \min_y \{ \|y\|_2 : Ay = b \}$$

For that, we can use SVD:

Theorem (SVD) $\quad A \in \mathbb{R}^{m \times n} \Rightarrow \exists\, \sigma_1 \geq \ldots \geq \sigma_{\min(m,n)}$

and $\exists$ orthog. mat. $U \in \mathbb{R}^{m \times m}$, $V \in \mathbb{R}^{n \times n}$,

Σ with $\Sigma_{ij} = \delta_{ij}\sigma_i$ st.

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

$\Rightarrow$ i) if all $\sigma_i = 0$ except for $\sigma_1, \ldots \sigma_r \Rightarrow r = \text{rank}(A)$

ii) the first r colums of U are an orthog. basis of $\text{Im}(A)$

iii) the colums $r+1, \ldots n$ of V - " - $\ker(A)$

$1, \ldots r$ of V - " - $(\ker(A))^\perp$

iv) the eigenvalues of A^TA are the eigenvalues of $\Sigma^T\Sigma$

Theorem (Min norm sol. of least squares problem) $\quad m \leq n$

Assume ~~A~~ $m = r$ (full rank) $\quad V = (\tilde{V}, V')$

$\tilde{\Sigma} := \Sigma_{1:r,\,1:r}$, $\quad \tilde{V} := V_{:,\,1:r}$, $\quad V' := V_{:,\,r+1:n}$

reduced SVD: $A = U \tilde{\Sigma} \underbrace{\tilde{V}^T}$ storing all non-zero entries!!

Define $\tilde{x} := \tilde{V} \tilde{\Sigma}^{-1} U^T b \quad \Rightarrow \tilde{x}$ solves $A\tilde{x} = b$,

since $A\tilde{x} = U \tilde{\Sigma} \tilde{V}^T \tilde{V} \tilde{\Sigma}^{-1} U^T b = b$.

Let $x := \tilde{x} + V'y$ be solution to $Ax = b$

$\Rightarrow$ min norm is attained for $y = 0$ $\quad (\|x\| = \|\tilde{x}\| + \|V'y\|)$

$\tilde{x}$.. min. norm. sol.

Def (Moore-Penrose Inverse) $\quad A^+ := \tilde{V} \tilde{\Sigma}^{-1} \tilde{U}^T$

Theorem $\quad$ The minim. norm solution to the least squ. problem can be found by $\tilde{x} = A^+ b$

(no conditions on m, n, r)

Proof: decompose: $b = \underbrace{\tilde{U}\tilde{U}^T b}_{\text{component in rang } A} + \underbrace{U'(U')^T b}_{\text{rest}}$ $\Big\}$ see lect. notes Lemma 5.25

For arbitrary $x \in \mathbb{R}^n$:

$$\|Ax-b\|_2^2 = \|\tilde{U}\tilde{\Sigma}\tilde{V}^T x - b\|^2 = \ldots = \|\tilde{\Sigma}V^T x - \tilde{U}^T b\|^2 + \|U'U'^T b\|$$

This is minimal for

$$\tilde{V}^T x = \tilde{\Sigma}^{-1}\tilde{U}^T b$$

Use again decomposition from Lemma 5.25:

$$\|x\|^2 = \|\tilde{V}\tilde{V}^T x\|^2 + \|V'V'^T x\|^2 \overset{\vee}{=} \|\tilde{V}\tilde{\Sigma}\tilde{U}^T b\|^2 + \|V'V'^T x\|^2$$

$\Rightarrow$ x with smallest norm satisfies $V'^T x = 0$

and we get $x = \tilde{V}\tilde{\Sigma}^{-1}\tilde{U}^T b = A^+ b$ ∎

Interpretation

$$A^+ : b \mapsto \hat{U}\tilde{U}^T b \mapsto A_k^{-1}\tilde{U}\tilde{U}^T b = \underbrace{\tilde{V}\tilde{\Sigma}^{-1}\tilde{U}^T}_{=A^+} b$$

orthog. proj. onto range of A, ie. $\tilde{U}\tilde{U}^T$

inverse of orthogon. Kernel of A, ie.

$$A_k : (\mathrm{Ker}(A))^\perp \to \mathrm{Range}\, A$$
$$\tilde{V}z \mapsto A\tilde{V}z = \tilde{U}\tilde{\Sigma}z$$

Computing SVD

compute eigenvals + eigvec of $\begin{pmatrix} 0 & A^T \\ A & 0 \end{pmatrix}$

6, Nonlinear equations & Newton's method

goal: find x st. $f(x) = 0$

Newton method: linearize f: $L(x) := f(x_n) + f'(x_n)(x - x_n)$

x_{n+1} is zero of $L(x)$

$$\Rightarrow \quad x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} =: \phi^{Newton}(x_n)$$

This is a fixed point iteration, as the zero of f (x^*) yields $x^* = \phi(x^*)$

Definition (Contraction) $\phi: \mathbb{R}^d \to \mathbb{R}^d$ is a contr. wrt. $\|\cdot\|$ if $\exists\, q \in (0,1)$ st.

$$\|\phi(x) - \phi(y)\| \le q\|x - y\| \quad \text{after some iterations}$$