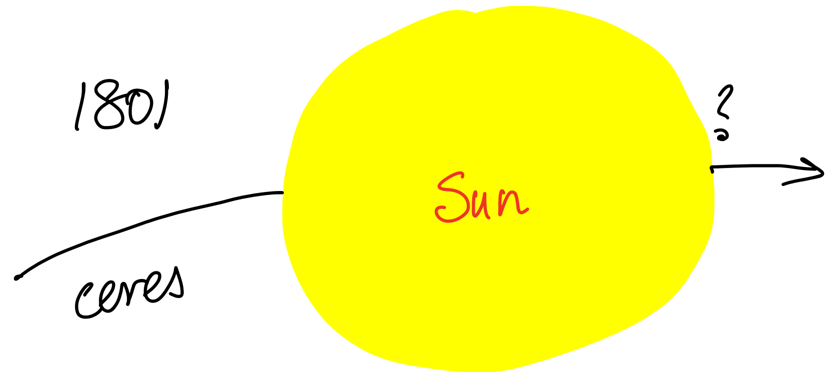
Least Squares Problem

History: Gauss



- attempt to obtain trajectory of Ceres
- without solving Kepler's equations
- Gauss used L.S.

$$\min_x \|Ax-b\|_2^2 = \min_x x^T A^T A x + 2b^T A x + b^T b$$

$$A^T A \succeq 0 \qquad \text{(QP)}$$

$x \in \mathbb{R}^n$
$b \in \mathbb{R}^m$

(a) $b \in R(A) \Rightarrow \exists x$ s.t. $Ax = b$

$$\Rightarrow \min \|Ax-b\|_2^2 = 0$$

(b) $b \notin R(A)$ $\quad \nabla \ell(x) = 0$

$$\Leftrightarrow 2A^TAx = 2A^Tb$$

$$x = \underbrace{(A^TA)^{-1}}_{\text{when exists}} A^Tb$$

Eg: $A = \begin{bmatrix} 1 & 2 \\ 1 & 2 \\ 1 & 2 \end{bmatrix}$ $\quad A^TA = \begin{bmatrix} 3 & 6 \\ 6 & 12 \end{bmatrix}$

solution to $(A^TA)x = A^Tb$
not unique

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

Then $\|b - Ax\|_2^2 = \|b - U\Sigma \underbrace{V^Tx}\|_2^2$

$\hat{x} = V^Tx$

$x = V\hat{x}$

$$= \|b - U\Sigma\hat{x}\|_2^2$$

Aside: $\|Ua\| = \|a\|$

since $\|Ua\|_2^2 = a^TU^TUa = a^Ta = \|a\|^2$

$$= \|U^Tb - U^TU\Sigma\hat{x}\|_2^2$$

$$= \|U^Tb - \Sigma\hat{x}\|$$

denote $U^T b = \tilde{b}$

$$\min_{\tilde{x}} \|\tilde{b} - \Sigma \tilde{x}\|_2^2$$

$\tilde{x} \in \mathbb{R}^n$
$\tilde{b} \in \mathbb{R}^m$
$\Sigma \in \mathbb{R}^{m \times n}$

$$= \min_{\tilde{x}} \left\| \begin{bmatrix} \tilde{b}_1 - \sigma_1 \tilde{x}_1 \\ \tilde{b}_2 - \sigma_2 \tilde{x}_2 \\ \vdots \\ \tilde{b}_r - \sigma_r \tilde{x}_r \\ \tilde{b}_{r+1} \\ \vdots \\ \tilde{b}_m \end{bmatrix} \right\|_2^2$$

rank(A)

$$\min_{\{\tilde{x}_i\}_{i=1}^{r}} \sum_{i=1}^{r} (\tilde{b}_i - \sigma_i \tilde{x}_i)^2 + \sum_{i=r+1}^{m} \tilde{b}_i^2$$

$\tilde{x}_{r+1} \dots \tilde{x}_m$ do not effect objective

$\tilde{x}_i = \tilde{b}_i / \sigma_i \quad i = 1 \dots r$

$\sigma_i > 0$

$\tilde{x}_i$ arbitrary $\quad i = r+1 \dots m$

$$\tilde{x} = \Sigma^+ \tilde{b} \quad \text{where} \quad [\Sigma^+]_{ii} = \begin{cases} 1/\sigma_i & i = 1 \dots r \\ 0 & \text{o/w} \end{cases}$$

$$x = \underbrace{V \Sigma^+ U^T}_{\text{pseudo inverse}} b$$