Linear Least Squares Supplement

FP Ch22

Consider a system of p linear equations in q unknowns

$$a_{11}x_1 + a_{12}x_2 + \cdots + a_{1q}x_q = y_1$$
$$a_{21}x_1 + a_{22}x_2 + \cdots + a_{2q}x_q = y_2$$
$$\vdots$$
$$a_{p1}x_1 + a_{p2}x_2 + \cdots + a_{pq}x_q = y_p$$

or $\quad A \quad x = \quad b$

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1q} \\ \vdots & & \ddots & \vdots \\ a_{p1} & & \cdots & a_{pq} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_q \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_p \end{bmatrix}$$

or $[c_1 \cdots\cdots c_q] \rightarrow$ columns

$p < q$ set of solutions forms a $(q-p)$-dimensional vector subspace of $\mathbb{R}^q$

Gaussian Elimination] $p = q$ unique solution

$p > q$ no solution

All true in the case that $\mathrm{rank}(A) = \min(p,q)$

Consider the overconstrained case $p > q$
and assume $\mathrm{rank}(A) = q$.

No exact solution, so we seek one that minimizes the
error measure

$$E(x) \doteq \sum_{i=1}^{p} (a_{i1}x_1 + \cdots + a_{iq}x_q - y_i)^2$$

$$= \|Ax - y\|^2 \quad , \quad \|\cdot\| \text{ Euclidean norm}$$

This is a linear least-squares problem.
→ E is proportional to the mean-squared error
with the equations, and each term is linear
before squaring.

Solve $e \doteq Ax - y$, $E = e e$ $\qquad 2e \frac{\partial e}{\partial x_i}$

$$\frac{\partial E}{\partial x_i} = 2 \frac{\partial e}{\partial x_i} \cdot e = 0 \quad , \text{for } i = 1, \ldots, q$$

$$\frac{\partial e}{\partial x_i} = \frac{\partial}{\partial x_i} (x_1 c_1 + \cdots x_q c_q - y) = \underline{c_i}$$

column i of A

$$\text{So, } \frac{\partial E}{\partial x_i} = 0 \Rightarrow \underline{c_i}^T (Ax - y) = 0$$

Stacking these constraints for each q coordinates of x

$$0 = \begin{pmatrix} c_1^T \\ \cdots \\ c_q^T \end{pmatrix}(Ax-y) = A^T(Ax-y)$$

the "normal equations" for our problem

$$\Updownarrow$$

$$A^TAx = A^Ty$$

When A has maximal rank q, A^TA is invertible

$$x = \underbrace{(A^TA)^{-1}A^T}_{A^+}y$$

$A^+ \longrightarrow$ the "pseudo inverse"

$$\boxed{A^+ = (A^TA)^{-1}A^T}$$