최소자승법 및 곡선맞춤

측정 Data :

$(x_1, y_1), (x_2, y_2), \cdots, (x_n, y_n)$

위의 Data를 가장 표현할 수 있는 다음과 같은 곡선을 생각하자.

$$g(x) = c_1 f_1(x) + c_2 f_2(x) + \cdots + c_m f_m(x)$$

여기서, $f_1(x), \cdots, f_m(x)$ 는 주어진 함수이다.

예) $f_k(x) = x^{k-1}$

문제1) $g(x_i) = y_i, \quad i = 1, 2, \cdots, n$ 인

$c_1, c_2, \cdots, c_m$ 을 찾을 수 있는가?

Ans) $n > m$ 일 때 일반적으로 찾을 수 없다.

문제2) $g(x_i) \approx y_i$ 인 c_i 를 찾아보자.

Ans) $g(x_i) \approx y_i$ 라는 것은 $g(x)$ 가 측정 Data

근처를 지난다는 의미로 그 Data의 분포는

$y = g(x)$ 를 따른다고 볼 수 있다.

이 때, $y = g(x)$ 는 측정 Data 의 맞춤 곡선이라 한다.

문제 3) 맞춤 곡선은 하나인가?

No) $f_i(x)$ 를 선택함에 따라 무수히 많다.

Data의 분포에 따라 $f_i(x)$ 를 선택

또한, 추정 방법에 따라 $g(x)$ 가 달라 질 수 있다.

< Least-squares with special functions >

Let $x = (x_i)_m$, $y = (y_i)_m$ be a data and

let $\mathcal{B} = \mathrm{span}(\phi_1, \phi_2, \cdots, \phi_n)$ be a function space based on some functions ϕ_i'.

Find a function $g \in \mathcal{B}$:

$$g(x) = \sum_{k=1}^{n} a_k \phi_k = a_1 \phi_1(x) + a_2 \phi_2(x) + \cdots + a_n \phi_n(x)$$

which minimizes

$$F(g) = \sum_{i=1}^{m} |g(x_i) - y_i|^2 .$$

* g can be a function of $a_1, a_2, \cdots, a_n$
* $F(g)$ is indeed a function of $a_1, a_2, \cdots, a_n$
* That is, the unknowns are $a_1, a_2, \cdots, a_n$

$$F(g) = \sum_{i=1}^{m} |g(x_i) - y_i|^2$$

$$\Rightarrow F(a_1, \cdots, a_n) = \sum_{i=1}^{m} \left| \sum_{k=1}^{n} a_k \phi_k(x_i) - y_i \right|^2$$

From $\dfrac{\partial F}{\partial a_j} = 0$ for $j = 1, 2, \cdots, n$

$$\cancel{2} \sum_{i=1}^{m} \left(\sum_{k=1}^{n} a_k \phi_k(x_i) - y_i \right) \phi_j(x_i) = 0$$

$$\Rightarrow \sum_{k=1}^{n} a_k \left(\sum_{i=1}^{m} \phi_k(x_i) \phi_j(x_i) \right) = \sum_{i=1}^{m} \phi_j(x_i) y_i .$$

Hence, the j-th row is given by

$$\left[\sum_{i=1}^{m} \phi_j(x_i)\phi_1(x_i) \quad \sum_{i=1}^{m} \phi_j(x_i)\phi_2(x_i) \quad \cdots \quad \sum_{i=1}^{m} \phi_j(x_i)\phi_n(x_i) \right] \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} = \left[\sum_{i=1}^{m} \phi_j(x_i) y_i \right]$$

Hence the system is given by

$$\begin{bmatrix} \sum_{i=1}^{m} \phi_1(x_i)\phi_1(x_i) & \sum_{i=1}^{m} \phi_1(x_i)\phi_2(x_i) & \cdots & \sum_{i=1}^{m} \phi_1(x_i)\phi_n(x_i) \\ \sum_{i=1}^{m} \phi_2(x_i)\phi_1(x_i) & \sum_{i=1}^{m} \phi_2(x_i)\phi_2(x_i) & \cdots & \sum_{i=1}^{m} \phi_2(x_i)\phi_n(x_i) \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^{m} \phi_n(x_i)\phi_1(x_i) & \sum_{i=1}^{m} \phi_n(x_i)\phi_2(x_i) & \cdots & \sum_{i=1}^{m} \phi_n(x_i)\phi_n(x_i) \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{m} \phi_1(x_i) y_i \\ \sum_{i=1}^{m} \phi_2(x_i) y_i \\ \vdots \\ \sum_{i=1}^{m} \phi_n(x_i) y_i \end{bmatrix}$$

$$A^T A u = A^T Y$$: normal equation

$$\underbrace{\begin{bmatrix} \phi_1(x_1) & \phi_2(x_1) & \cdots & \phi_n(x_1) \\ \phi_1(x_2) & \phi_2(x_2) & \cdots & \phi_n(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(x_m) & \phi_2(x_m) & \cdots & \phi_n(x_m) \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}}_{u} = \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}}_{Y}$$

$A_{ij} = \phi_j(x_i)$: $m \times n$ matrix.

<Example>

Find a fitting function

$$g(x) = a_1 \sin(\pi x) + a_2 \cos(\pi x) + a_3 \pi x$$

on $[0, 1]$

for the data

$$\left(\frac{1}{6}, 1\right), \left(\frac{1}{4}, 0\right), \left(\frac{1}{2}, -1\right), \left(\frac{3}{4}, 0\right).$$

Let $\phi_1 = \sin \pi(x)$, $\phi_2 = \cos \pi x$, $\phi_3 = \pi x$.

$$A = (A_{ij}) = \phi_j(x_i).$$

$$u = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}, \quad Y = \begin{bmatrix} 1 \\ 0 \\ -1 \\ 0 \end{bmatrix} \quad X = \begin{bmatrix} \frac{1}{6} \\ \frac{1}{4} \\ \frac{1}{2} \\ \frac{3}{4} \end{bmatrix}$$

$$\Rightarrow A = \begin{bmatrix} \phi_1(X) & \phi_2(X) & \phi_3(X) \end{bmatrix}$$

Exa 1) 선형 맞춤 (Regression line : 회귀 직선)

$f_1(x) = x, \quad f_2(x) = 1.$

$$A = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_m & 1 \end{bmatrix}, \quad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}$$

Exa 2) 거듭제곱 함수에 의한 맞춤 : $g(x) = \beta x^{\alpha}$

$y_i \approx \beta x_i^{\alpha}$ 에서

$\log y_i \approx \alpha \log(x_i) + \log(\beta)$

Set $Y_i = \log y_i, \quad X_i = \log(x_i)$

$c_1 = \alpha, \quad c_2 = \log(\beta)$

$\rightarrow \quad Y_i \approx c_1 X_i + c_2.$

$$A = \begin{bmatrix} X_1 & 1 \\ \vdots & \vdots \\ X_m & 1 \end{bmatrix} = \begin{bmatrix} \log x_1 & 1 \\ \vdots & \vdots \\ \log x_m & 1 \end{bmatrix}, \quad Y = \begin{bmatrix} \log y_1 \\ \vdots \\ \log y_m \end{bmatrix}$$

c_1과 c_2를 찾은 다음 $\alpha = c_1, \quad \beta = e^{c_2}$

Exa 3) 고차다항식에 의한 맞춤

$$g(x) = c_1 x^n + c_2 x^{n-1} + \cdots + c_n x + c_{n+1}.$$

i.e) $f_i(x) = x^{n-i+1}$

$$A = \begin{bmatrix} x_1^n & x_1^{n-1} & \cdots & 1 \\ x_2^n & x_2^{n-1} & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ x_m^n & x_m^{n-1} & \cdots & 1 \end{bmatrix}, \quad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}$$

Exa 4) 함수들의 선형조합.

$$g(x) = c_1 + c_2 x + c_3 \sin x + c_4 \exp(x)$$

$$A = \begin{bmatrix} 1 & x_1 & \sin x_1 & \exp(x_1) \\ 1 & x_2 & \sin x_2 & \exp(x_2) \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_m & \sin x_m & \exp(x_m) \end{bmatrix}, \quad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}$$

Exa 5) 퓰리에 맞춤

$$g(x) = c_1 \sin x + c_2 \sin 2x + \cdots + c_m \sin mx$$