

最小二乘法

参数(未知)个数 < 方程(点)个数:

如, 已知 ~~n~~ (n+1) 个点 $(x_i, y_i) (i=0, \dots, n)$

多项式: $y = a_0 + a_1 x + \dots + a_m x^m$ (m+1 参数), 且 $m < n$.

建立方程组:

$$\left. \begin{aligned} a_0 + a_1 x_0 + \dots + a_m x_0^m - y_0 &= \delta_0 \\ \dots & \\ a_0 + a_1 x_n + \dots + a_m x_n^m - y_n &= \delta_n \end{aligned} \right\} \text{n+1 个方程}$$

($\delta_0, \delta_1, \dots, \delta_n$ 表示误差)

我们的目标是找到 (a_0, a_1, \dots, a_m) , 使得 $\sum_{i=0}^n \delta_i^2$ 最小. (以致 $|\delta_i|$ 很小)

令 $A = (x_i^j)_{(n+1) \times (m+1)}$ ($i=0, \dots, n; j=0, \dots, m$)

$a = (a_0, a_1, \dots, a_m)_{1 \times (m+1)}^T$

$y = (y_0, y_1, \dots, y_n)_{1 \times (n+1)}^T$

$\delta = (\delta_0, \delta_1, \dots, \delta_n)_{1 \times (n+1)}^T$

则 $A \cdot a - y = \delta$, 求 a 使 $\|\delta\|$ 最小.

其中 $\|\delta\|^2 = [Aa - y]^T \cdot [Aa - y]$, 视为 $f(a)$, 对 a 求导. (*)

$a^T \cdot A \cdot a - a^T y = 0$.

可证 $|a^T \cdot a| > 0$.

$\therefore a = (a^T \cdot a)^{-1} \cdot a^T y$.

找系数矩阵 $G = (A^T A)^{-1} A^T$
(n+1) x (m+1)

(*) : 对求导的补充. 设 $f(a) = [Aa - y]^T [Aa - y] = \sum_{i=0}^n (\sum_{j=0}^m x_i^j a_j - y_i)^2$

则 $\frac{\partial f}{\partial a_k} = \sum_{i=0}^n 2 \cdot (\sum_{j=0}^m x_i^j a_j - y_i) \cdot x_i^k$, 令 $\frac{\partial f}{\partial a_k} = 0$

则 $\sum_{i=0}^n (\sum_{j=0}^m x_i^j a_j) x_i^k - \sum_{i=0}^n y_i x_i^k = 0$ ($k=0, 1, \dots, m$)

~~即 $\sum_{i=0}^n \sum_{j=0}^m x_i^j a_j x_i^k - \sum_{i=0}^n y_i x_i^k = 0$~~

把方程组按列排列有 $A^T A \cdot a - A^T y = 0$