线性回归闭式解推导

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1 基本概念

1、线性模型

$$f_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + ... + \theta_n x_n$$

矩阵形式为：

$$f(x) = \sum_{i=0}^{n} \theta_i x_i = \theta^T x$$

2、目标函数

由于

$$z^T z = \sum_i z_i^2$$

所以损失函数可写为：

$$J(\theta) = \frac{1}{2} \sum_{i=0}^{m} (f_\theta(x^{(i)} - y^{(i)})^2) = \frac{1}{2} (X\theta - y)^T (X\theta - y)$$

2 闭式解推导

基本性质

$$trA = \sum_{i=1}^{n} A_{ii}$$

$$trAB = trBA$$

$$trA = trA^T$$

$$tr(real) = real$$

$$\nabla_A trAB = B^T$$

$$\nabla_{A^T} f(A) = (\nabla_A f(A))^T$$

$$\nabla_A trABA^T C = CAB + C^T AB^T$$

$$\nabla_A |A| = |A|(A^{-1})^T$$

$$\nabla_{A^T} trABA^T C = (\nabla_A trABA^T C)^T = (CAB + C^T AB^T)^T = B^T A^T C^T + BA^T C$$

推导过程

$$
\begin{aligned}
\nabla_\theta J(\theta) &= \nabla_\theta \frac{1}{2}(X\theta - y)^T(X\theta - y) \\
&= \frac{1}{2}\nabla_\theta(\theta^T X^T X\theta - \theta^T X^T y - y^T X\theta + y^T y) \\
&= \frac{1}{2}\nabla_\theta tr(\theta^T X^T X\theta - \theta^T X^T y - y^T X\theta + y^T y) \\
--> trA^T = trA => tr(\theta^T X^T y) = tr(y^T X\theta) \\
&= \frac{1}{2}\nabla_\theta(tr\theta^T X^T X\theta - 2tr(y^T X\theta)) \\
--> (\theta = A^T, B = X^T X, C = I) \\
&= \frac{1}{2}\nabla_{A^T}(tr(ABA^T C)) - \frac{1}{2}\nabla_\theta 2tr(y^T X\theta) \\
&= \frac{1}{2}(B^T A^T C^T + BA^T C) - X^T y \\
&= \frac{1}{2}(X^T X\theta + X^T X\theta) - X^T y \\
&= X^T X\theta - X^T y
\end{aligned} \tag{1}
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于是令 $\nabla_\theta J(\theta) = 0$ 得到 $X^T X\theta = X^T y$, 于是:

$$\theta = (X^T X)^{-1} X^T y$$

上式即为 θ 的闭式解。