读书报告

第三章 线性模型

刘精昌

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引例

工资与教育水平关系

考查工人工资水平与其受教育关系:

a 工资水平(每小时美元数):用 Y 表示

b 受教育程度(受教育年数):用 X 表示

c 非可观测因素,如工作经验、天生素质、工作时间等其他因素

引例

工资与教育水平关系

- 观测的数据：(x_i, y_i) , $i = 1, \cdots, n$ （受访人数），

i	x_i	y_i	i	x_i	y_i
1	5.3	1.4	9	8.5	3.2
2	11.0	3.9	10	7.1	8.6
3	9	6.3	11	15	4
4	8.7	8.6	12	12.0	9.0
5	10	12	13	29	12
6	15.5	12	14	19.7	13.1
7	21	16	15	15.1	10
8	19	14.4	16	15.7	16

定义

$$y_i = \beta_0 + x_{i1}\beta_1 + \cdots + x_{i,p-1}\beta_{p-1} + e_i,\ i = 1, 2, \ldots, n$$

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} 1 & x_{11} & \cdots & x_{1,p-1} \\ 1 & x_{11} & \cdots & x_{2,p-1} \\ \vdots & \vdots & & \vdots \\ 1 & x_{11} & \cdots & x_{n,p-1} \end{pmatrix} \begin{pmatrix} \omega_0 \\ \omega_1 \\ \vdots \\ \omega_{p-1} \end{pmatrix} + \begin{pmatrix} e_1 \\ e_2 \\ \vdots \\ e_{p-1} \end{pmatrix}$$

$$\mathbf{y} = \mathbf{X}\beta + \mathbf{e}$$

$$y_i = \beta_0 + x_{i1}\beta_1 + \cdots + x_{i,p-1}\beta_{p-1} + e_i,\ i = 1, 2, \ldots, n$$

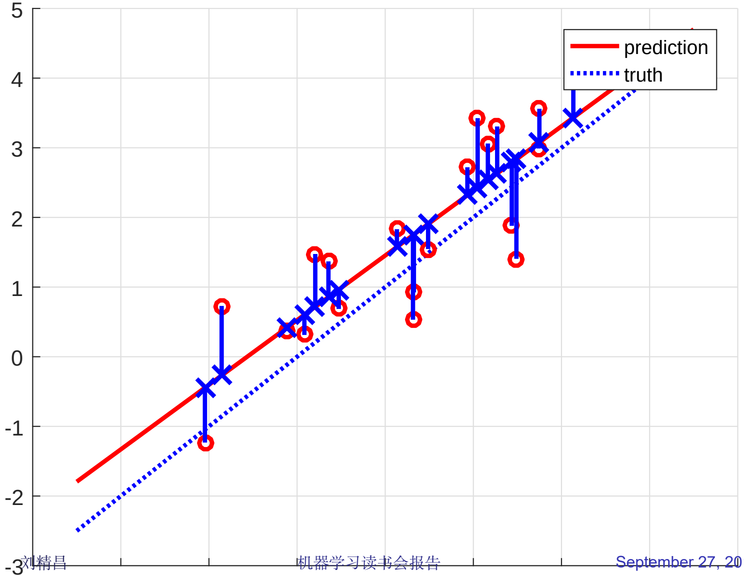
(a) 拟合值：$\hat{y}_i = \hat{\beta}_0 + x_{i1}\hat{\beta}_1 \cdots + x_{i,p-1}\hat{\beta}_{p-1}$

(b) 残差（residual）:$\varepsilon_i = y_i - \hat{y}_i = y_i - \hat{\beta}_0 - x_{i1}\hat{\beta}_1 \cdots + x_{i,p-1}\hat{\beta}_{p-1}$

(c) 残差平方和（residual sum of squares RSS）

$$RSS(\beta) = \sum_{i=1}^{n} {\varepsilon_i}^2 = \sum_{i=1}^{n} \left(y_i - \hat{y}_i\right)^2 = \left(\hat{y} - X\hat{\beta}\right)^T \left(\hat{y} - X\hat{\beta}\right)$$

残差示意图



参数求解

最小二乘法：RSS 最小

1. $E(\overset{\wedge}{\beta}) = \left(y - X\overset{\wedge}{\beta}\right)^T \left(y - X\overset{\wedge}{\beta}\right) = y^T y - 2y^T X\overset{\wedge}{\beta} + \overset{\wedge}{\beta}^T X^T X\overset{\wedge}{\beta}$
2. $\dfrac{\partial E\left(\overset{\wedge}{\beta}\right)}{\partial \overset{\wedge}{\beta}} = 0$
3. $X^T X\overset{\wedge}{\beta} = X^T y$
4. $\overset{\wedge}{\beta} = (X^T X)^{-1} X^T y$

MLE

1. $y_i = \beta^T x_i + e_i, e_i \sim N\left(0, \sigma^2\right)$
2. $y_i \sim N\left(\beta^T x_i, \sigma^2\right)$
3. $\overset{\wedge}{\beta} \triangleq \arg\max_{\beta} \log p\left(D \,|\beta\right)$
4. $l\left(\beta\right) \triangleq \log p\left(D \,|\beta\right) = \sum_{i=1}^{n} \log p\left(y_i \,|\beta\right) = \sum_{i=1}^{n} \log\left[\left(\frac{1}{2\pi\sigma^2}\right)^{\frac{1}{2}} \exp\left(-\frac{1}{2\sigma^2}\left(y_i - \beta^T x_i\right)^2\right)\right] = -\frac{1}{2\sigma^2} RSS - \frac{N}{2} \log\left(2\pi\sigma^2\right)$

平方和的定义

a、 总平方和 (Total Sum of Squares TSS):

$$TSS \triangleq \sum_{i=1}^{n} (y_i - \overline{y})^2, \overline{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$$

b、 解释平方和（Explained Sum of Squares ESS）:

$$ESS \triangleq \sum_{i=1}^{n} \left(\hat{y}_i - \overline{\hat{y}}\right)^2, \overline{\hat{y}} = \frac{1}{n}\sum_{i=1}^{n} \hat{y}_i$$

- TSS = ESS + RSS

拟合优度

判定系数的定义

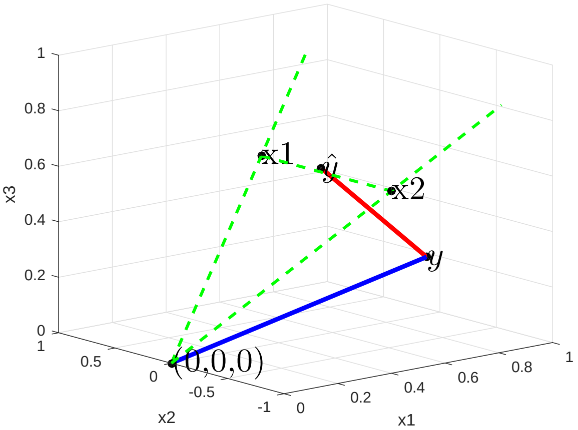
$$R^2 = \frac{ESS}{TSS}$$

判定系数的性质

- $0 \leq R^2 \leq 1$
- R^2 越接近 1，拟合效果越好
- R^2 越接近 0，拟合效果越差

几何解释

$$\hat{y} = X\hat{\beta} = X\left(X^TX\right)^{-1}X^Ty$$



增加惩罚项

ridge regression

- $J(\beta) = \frac{1}{n} RSS + \lambda \|\beta\|_2^2$
- $\underset{ridge}{\overset{\wedge}{\beta}} = \min_{\beta} \arg J(\beta)$
- $\underset{ridge}{\overset{\wedge}{\beta}} = \left(\lambda I + X^T X\right)^{-1} X^T y$

LASSO

$$J(\beta) = \frac{1}{n} RSS + \lambda \|\beta\|_1$$

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定义

$$p\left(y\left|x,w\right.\right)=Ber\left(y\left|sigm\left(w^{T}x\right)\right.\right)=\begin{cases} sigm\left(w^{T}x\right),y=1\\ 1-sigm\left(w^{T}x\right),y=0\end{cases}$$

$$sigm\left(w^{T}x\right)=\frac{1}{1+e^{w^{T}x}}$$

sigmoid 示意图

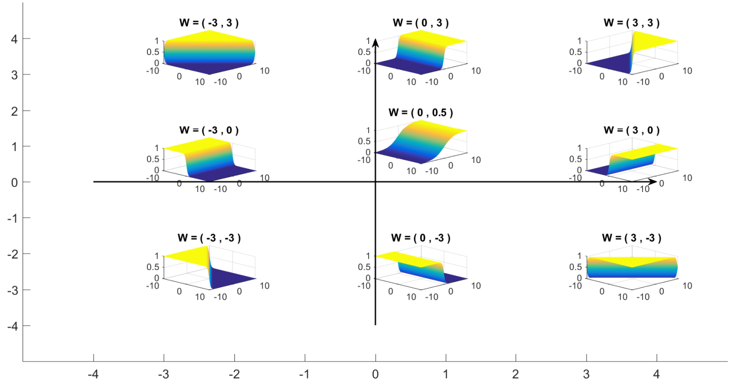

Figure: sigmoid 示意图

MLE

$$\mu_i = sigm\left(w^T x_i\right) = \frac{1}{1 + e^{w^T x_i}}$$

$$\begin{aligned} NLL(w) &= -\sum_{i=1}^{N} \log\left(\mu_i^{\mathrm{I}(y_i=1)} \times (1-\mu_i)^{\mathrm{I}(y_i=0)}\right) \\ &= -\sum_{i=1}^{N} \left[y_i \log \mu_i + (1-y_i)\log(1-\mu_i)\right] \end{aligned}$$

MLE

$$\frac{\partial \mu_i}{\partial w} = -\frac{x_i e^{w^T x_i}}{\left(1 + e^{w^T x_i}\right)^2} = -x_i \mu_i \left(1 - \mu_i\right)$$

$$\begin{aligned} \frac{\partial NLL\left(w\right)}{\partial w} &= \sum_{i=1}^{N} \frac{\partial NLL\left(w\right)}{\partial \mu_i} \frac{\partial \mu_i}{\partial w} \\ &= \sum_{i=1}^{N} \left(\frac{y_i}{\mu_i} - \frac{1 - y_i}{1 - \mu_i} \right) x_i \mu_i \left(1 - \mu_i\right) \\ &= \sum_{i=1}^{N} \left(x_i y_i - x_i \mu_i\right) \\ &= X^T \left(\mu - y\right) \end{aligned}$$

$$H = \frac{\partial^2 NLL\left(w\right)}{\partial w^2} = -X^T S X, S \triangleq diag\left(\mu_i \left(1 - \mu_i\right)\right)$$

Optimization

Steepest descent

$$\theta_{k+1} = \theta_k - \eta_k g_k$$

Newton's method

$$\theta_{k+1} = \theta_k - \eta_k H_k^{-1} g_k$$

softmax

$$\left\{\left(x^{(1)},y^{(1)}\right),\left(x^{(2)},y^{(2)}\right),\ldots,\left(x^{(n)},y^{(n)}\right)\right\},y^{(i)}\in\{1,2,\ldots,k\}$$

$$\begin{bmatrix} p\left(y^{(i)}=1\left|x^{(i)};\theta\right.\right) \\ p\left(y^{(i)}=2\left|x^{(i)};\theta\right.\right) \\ \vdots \\ p\left(y^{(i)}=k\left|x^{(i)};\theta\right.\right) \end{bmatrix} = \frac{1}{\sum_{j=1}^{k} e^{w_j^T x^{(i)}}} \begin{bmatrix} e^{w_1^T x^{(i)}} \\ e^{w_2^T x^{(i)}} \\ \vdots \\ e^{w_k^T x^{(i)}} \end{bmatrix}$$

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LDA 示意图

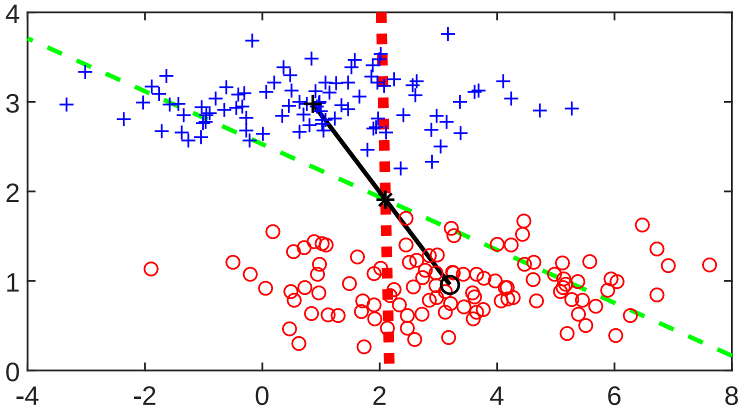

Figure: LDA 示意图

LDA

$$J(w) = \frac{w^T S_B w}{w^T S_W w}$$

- between-class scatter matrix

$$S_B = (\mu_2 - \mu_1)(\mu_2 - \mu_1)^T$$

- within-class scatter matrix

$$S_W = \sum_{i:y_i=1} (x_i - \mu_1)(x_i - \mu_1)^T + \sum_{i:y_i=2} (x_i - \mu_2)(x_i - \mu_2)^T$$

求解

1. $J^{'}(w) = w^T S_B w - \lambda w^T S_W w, \lambda > 0$
2. $\frac{dJ^{'}(w)}{dw} = 0$
3. $\lambda S_w w = S_B w$
4. $S_B w = (\mu_2 - \mu_1)(\mu_2 - \mu_1)^T w = (\mu_2 - \mu_1)(m_2 - m_1)$
5. $w \propto S_w^{-1}(\mu_2 - \mu_1)$

Q & A