

## Lecture 5: Linear Models with Categorical predictors

*Lecturer: Prof. Jingyi Jessica Li**Subscribers: Narek Manoukian, Mina Shahi*

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## Tips for Homework 1

Generalized form of Wald Test:

If  $A$  is known to be an  $n \times p$  matrix

$$H_0 \rightarrow A\beta = 0$$

$$H_1 \rightarrow A\beta \neq 0$$

$$\text{Test statistic: } W = (A\hat{\beta})^T \cdot (\text{Var}(A\hat{\beta}))^{-1} \cdot (A\hat{\beta}) \xrightarrow{n \rightarrow \infty} \chi_m^2$$

Distribution of RSS(SSE)

$$RSS = \sum_{i=1}^n r_i^2 = r^T r$$

where  $r = (I - H)Y$  and  $Y = X\beta + \epsilon$ 

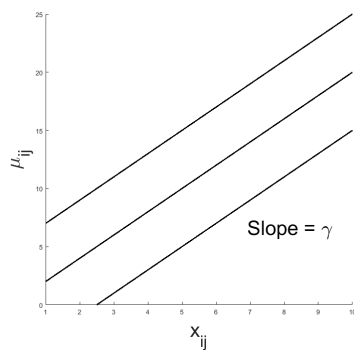
$$RSS = Y^T(I - H)Y = \epsilon^T(I - H)\epsilon$$

$$\frac{RSS}{\sigma^2} = (\epsilon/\sigma)^T(I - H)(\epsilon/\sigma) \sim \chi_{n-p}^2 \text{ where } (\epsilon/\sigma) \sim N(0, I_n) \text{ and rank } (I - H) = (n - p)$$

## 5.1 Analysis of Covariance Models

- Combination of categorical factors and continuous variables.
- $x$  continuous with 1 degree of freedom,  $z$  categorical with  $I$  levels and  $I - 1$  degrees of freedom.
- $n_i$  observations in level  $i$  of  $z$ .  $n = \sum_{i=1}^I n_i$ .
- Random structure:  $Y_{ij} \sim N(\mu_{ij}, \sigma^2)$ ,  $i = 1, \dots, I$ ;  $j = 1, \dots, n_i$
- Systematic structure:  $\mu_{ij} = \mu + \alpha_i + \gamma x_{ij}$  (i.e., additive model). Impose  $\alpha_1 = 0$  for identifiability.

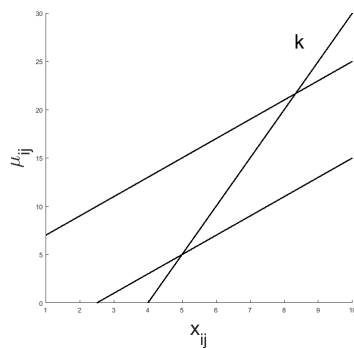
The parameters are  $\beta = (\mu, \alpha_2, \dots, \alpha_I, \gamma)^T$ .



Then this model represents  $I$  parallel lines, one for each group. The  $X$  matrix will look like

$$\begin{pmatrix}
 1 & \alpha_2 & \alpha_3 & \dots & \alpha_I & \gamma \\
 1 & 0 & 0 & \dots & 0 & x_{11} \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 1 & 0 & 0 & \dots & 0 & x_{1n_1} \\
 1 & 1 & 0 & \dots & 0 & x_{21} \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 1 & 1 & 0 & \dots & 0 & x_{2n_2} \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 1 & 0 & 0 & \dots & 1 & x_{I1} \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 1 & 0 & 0 & \dots & 1 & x_{In_I}
 \end{pmatrix}$$

We can drop the parallel lines assumption. Then  $\mu_{ij} = \mu + \alpha_i + (\gamma + \eta_i)x_{ij}$ .



- Identifiability conditions:  $\alpha_1 = \eta_1 = 0$
- Design matrix  $X$ ? Homework question.
- Can test  $H_0 : \alpha_2 = \dots = \alpha_I = 0$  by Wald test, LRT, or hierarchical ANOVA.

## 5.2 Regression Diagnostics

Statistical modeling has three stages:

1. Formulate a model - include random-ness and assumption
2. Fit the model to data - Optimization procedure
3. Check the model - Run model diagnostics

### 5.2.1 Residual Diagnostics

Residuals may also be expressed as:

$$\begin{aligned}
 e &= Y - \hat{Y} \\
 &= Y - X\hat{\beta} \\
 &= Y - X(X^T X)^{-1} X^T Y \\
 &= Y - HY \\
 &= (I - H)Y.
 \end{aligned}$$

It can be easily shown that the matrix  $H$  is idempotent, i.e.  $H^2 = H$  and symmetric, so that  $H^T = H$ . Also,  $(I - H)^T = (I - H)$  and  $(I - H)^2 = (I - H)$ .

Furthermore, linearity of  $\mathbb{E}[\cdot]$  implies that

$$\begin{aligned}
 \mathbb{E}[e] &= \mathbb{E}[(I - H)Y] \\
 &= (I - H)\mathbb{E}[Y] \\
 &= (I - H)X\beta \\
 &= X\beta - X(X^T X)^{-1} X^T X\beta \\
 &= 0.
 \end{aligned}$$

It also follows that:

$$\begin{aligned}
 \text{Var}[e] &= \text{Var}[(I - H)Y] \\
 &= \mathbb{E}[(I - H)YY^T(I - H)^T] - \mathbb{E}^2[(I - H)Y] \\
 &= (I - H)(\mathbb{E}[YY^T])(I - H)^T - 0 \\
 &= (I - H)\text{Var}[Y](I - H) \\
 &= (I - H)(\sigma^2 I)(I - H) \\
 &= \sigma^2(I - H)
 \end{aligned}$$

Hence,  $\text{Var}(e_i) = (1 - h_{ii})\sigma^2$ , so residuals do not have constant variance. However, note that  $\text{Var}(\varepsilon_i) = \sigma^2$ , the error terms have the same variance (constant variance assumption). Furthermore, we can also show that:

$$\begin{aligned}\text{tr}(H) &= \text{tr}(X(X^T X)^{-1} X^T) \\ &= \text{tr}(X^T X (X^T X)^{-1}) \\ &= \text{tr}(I_p) \\ &= p\end{aligned}$$

where  $p = \text{rank}(X)$ . Now by symmetry we have  $h_{ij} = h_{ji}$  which in combination with idempotency implies:

$$\begin{aligned}h_{ii} &= \sum_{j=1}^n h_{ij}^2 \\ &= h_{i1}^2 + \cdots + h_{ii}^2 + \cdots + h_{in}^2 \\ &\geq h_{ii}^2\end{aligned}$$

which is only possible if  $h_{ii} \in [0, 1]$ .

Hence,  $\text{Var}(e_i) = (1 - h_{ii})\sigma^2$ , so residuals do not have the same variance. Thus,  $\text{Var}(e_i) > 0$ , as  $h_{ii} < 1$ . And we can also see that larger the  $h_{ii}$ , smaller the  $\text{Var}(e_i)$ .

We can also show  $h_{ii} > 0$ , thus  $\text{Var}(e_i) < \text{Var}(\varepsilon_i) = \sigma^2$  given the error terms have the same variance (constant variance assumption).

**Ex** When  $p = 1$  (simple linear model):

$$X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}$$

$$h_{ii} = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum_{i'=1}^n (x_{i'} - \bar{x})^2}, \text{ where } \bar{x} = \frac{1}{n} \sum_{i=1}^n x_i.$$

Setting  $x_i = \bar{x}$  minimizes  $h_{ii}$  and maximizes  $\text{Var}(e_i)$ , here the minimum value of  $h_{ii}$  is  $\frac{1}{n}$ .

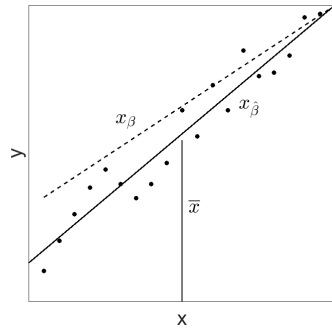
When  $x_i$  is far from  $\bar{x}$ ,  $\text{Var}(e_i)$  is small since  $h_{ii}$  is large. That is, a point farther away from the mean value has more impact on fitting the line, so the variance of its residual will be smaller, but variance of a residual around  $\bar{x}$  is larger because the data point has smaller impact on the fitted line.

**Definition 5.1** A standardized residual is defined as  $s_i = \frac{e_i}{\text{se}(e_i)} = \frac{e_i}{\sqrt{1 - h_{ii}}\hat{\sigma}} \sim N(0, 1)$ .

$$\text{where } \hat{\sigma}^2 = \frac{RSS}{n-p}$$

Look for observations that have  $|s_i| \geq 2$ . This is a rule of thumb for detecting potential outliers, but  $\hat{\sigma}$  itself may be influenced by outliers. This limits the use of standardized residuals.

Solutions



### 1. Jack knifed residual

Estimate  $\sigma$  from  $(n - 1)$  data points without using the  $i^{th}$  observation.

	Jack knifed Residuals (Tokey)	Bootstrap (Efron)
Computer	X	✓
Sample-size	n-1	n
Sampling	without replacement	with replacement
No. of samples	n	$\infty$

Book for reference: Jackknife and Bootstrap (1993) by Jon Shao

**Definition 5.2** The jackknifed residual is defined as  $t_i = \frac{e_i}{\sqrt{1 - h_{ii}}\hat{\sigma}_{(i)}}$

where  $\hat{\sigma}_{(i)}^2 = \frac{RSS_{(i)}}{n-p-1}$   
 $RSS_{(i)} \rightarrow$  residual sum of squares after leaving out the  $i$ -th observation.

$$\text{That is, } \hat{\sigma}_{(i)}^2 = \frac{\sum_{j \neq i}^n e_{(i)j}^2}{(n-1) - p}$$

To calculate all  $t_i$ 's, we don't need to do  $n$  regressions. By Weisberg (1985, p293),

$$t_i = s_i \sqrt{\frac{n-p-1}{n-p-s_i^2}},$$

where  $s_i = \frac{r_i}{\sqrt{1-h_{ii}}\hat{\sigma}}$ . As a result, one regression is enough and  $t_i$  is monotonic in  $s_i$ . Hence, ordering observations by  $s_i$  or by  $t_i$  will give the same rank.

### 2. Predictive residual ( $Y_i - \hat{Y}_{(i)}$ )

Let  $y_i - \hat{y}_{(i)}$  be the predicted value of the  $i^{th}$  observation without using the  $i^{th}$  observation in estimation of the regression line. The statistic  $y_i - \hat{y}_{(i)}$  is known as the predictive residual. Note that  $y_i$  and  $\hat{y}_{(i)}$  are independent, hence  $\text{Cov}[y_i, \hat{y}_{(i)}] = 0$ . It follows that:

$$\begin{aligned}\text{Var} [y_i - \hat{y}_{(i)}] &= \text{Var} [y_i] + \text{Var} [\hat{y}_{(i)}] \\ &= \sigma^2 + \text{Var} \left[ x_i^T (X_{(i)}^T X_{(i)})^{-1} X_{(i)}^T Y_{(i)} \right] \\ &= \sigma^2 + x_i^T (X_{(i)}^T X_{(i)})^{-1} X_{(i)}^T \text{Var} [Y_{(i)}] (x_i^T (X_{(i)}^T X_{(i)})^{-1} X_{(i)}^T)^T \\ &= \sigma^2 + \sigma^2 (x_i^T (X_{(i)}^T X_{(i)})^{-1} x_i)\end{aligned}$$