## What to do today (March 21, 2023)?

Part 3. Important Topics in Statistics (Chp 10-13)
§3.1. Analysis of Variance (ANOVA, Chp 10-11)
§3.2. Introduction to Regression Analysis (Chp 12-13)
§3.2.1 Introduction
§3.2.2 Simple Linear Regression (Chp 12)
§3.2.3 More Advanced Topics (Chp 13)

Some Logistics.

- Homework 9 has been assigned. It's due on Monday March 27.
- The remaining Midterm 2 papers are with Joan Hu.


### 3.2.2D Residual analysis

(model checking)

- (raw) Residual: $e_{i}=Y_{i}-\hat{Y}_{i}$ (observed - fitted) with $\hat{Y}_{i}=\hat{\beta}_{0}+\hat{\beta}_{1} X_{i}=\bar{Y}+\hat{\beta}_{1}\left(X_{i}-\bar{X}\right)$

$$
E\left(e_{i}\right)=0 ; \quad V\left(e_{i}\right)=\sigma^{2}\left[1-\frac{1}{n}-\frac{\left(X_{i}-\bar{X}\right)^{2}}{S_{X X}}\right]
$$

and $e_{i} \sim$ normal

- Standardized residual:

$$
e_{i}^{*}=e_{i} / s \sqrt{1-\frac{1}{n}-\frac{\left(X_{i}-\bar{X}\right)^{2}}{S_{X X}}}
$$

with $s^{2}=\hat{\sigma}^{2}=M S S_{e} . \Longrightarrow e_{i}^{*} \sim N(0,1)$ roughly

- Pearson residual: $\tilde{e}_{i}=e_{i} / s$ when $n \gg 1$ and $S_{X X} \gg\left(x_{i}-\bar{x}\right)^{2}, \tilde{e}_{i} \approx e_{i}^{*}$.


## Commonly-used diagnostic plots:

- $x_{i}$ vs $e_{i}$ (or $e_{i}^{*}$ or $\left.\tilde{e}_{i}\right)$
- $\hat{y}_{i}$ vs $e_{i}\left(\right.$ or $e_{i}^{*}$ or $\left.\tilde{e}_{i}\right)$
- $y_{i}$ vs $\hat{y}_{i}$
- a normal probability plot of $e_{i}$ (Z-percentile vs $e_{i}$ ):
- rank $e_{i}, i=1, \ldots, n$, denoted by

$$
e_{(1)}, \ldots, e_{(n)}
$$

- scatter plot:

$$
\left(Z_{1 / n-1 / 2 n}, e_{(1)}\right),\left(Z_{2 / n-1 / 2 n}, e_{(2)}\right), \ldots,\left(Z_{1-1 / 2 n}, e_{(n)}\right)
$$

Example 7.1 (cont'd) Consider a regression analysis under model $Y=\beta_{0}+\beta_{1} X+\epsilon$, assuming $\epsilon \sim N\left(0, \sigma^{2}\right)$ :

- (i) ANOVA

| Source of Variation | df | SS | MSS | F-value |
| :---: | :---: | :---: | :---: | :--- |
| regression | 1 | 398030.2 | $M S S_{\text {reg }}$ | $F_{\text {obs }}=\frac{M S S_{\text {reg }}}{M S S_{e}}=294.74$ |
| error | $n-2=12$ | 16205.45 | $M S S_{e}$ | $\gg F_{.95}(1,12)=3.17$ |
| total | $n-1=13$ | $S S_{T}$ |  |  |

$\left(S S_{T}=S S_{\text {reg }}+S S_{e}\right)$

- (ii) Test on $H_{0}: \beta_{1}=0$ vs $H_{1}: \beta_{1}>0$

$$
T=\frac{\hat{\beta}_{1}-0}{s_{\hat{\beta}_{1}}} \sim t(12) \text { under } H_{0}
$$

$$
T_{o b s}=1.711 / .0997=17.16 \gg t_{.95}(12)=1.78
$$

Example 7.1 (cont'd) Consider a regression analysis under model $Y=\beta_{0}+\beta_{1} X+\epsilon$, assuming $\epsilon \sim N\left(0, \sigma^{2}\right)$ :

- (iiia) Estimation for $E\left(Y \mid X=x^{*}\right)$ with $x^{*}=225$.

$$
\hat{Y} \mid x^{*}=\hat{\mu}_{Y \mid x^{*}}=\hat{\beta}_{0}+\hat{\beta}_{1} x^{*}=339.43
$$

$1-\alpha \mathrm{Cl}:$

$$
\hat{Y} \left\lvert\, x^{*} \pm t_{\alpha / 2}(n-2) \sqrt{M S S_{e}\left[\frac{1}{n}+\frac{\left(x^{*}-\bar{x}\right)^{2}}{S_{X X}}\right]} \Longrightarrow(317.90,360.95)\right.
$$

- (iiib) Prediction for $Y$ with $X=x^{*}=225$.

$$
\hat{y}^{*}=\hat{\beta}_{0}+\hat{\beta}_{1} x^{*}
$$

$1-\alpha$ prediction interval (PI)

$$
\hat{Y} \left\lvert\, x^{*} \pm t_{\alpha / 2}(n-2) \sqrt{M S S_{e}\left[1+\frac{1}{n}+\frac{\left(x^{*}-\bar{x}\right)^{2}}{S_{X X}}\right]} \Longrightarrow(256.51,422.34)\right.
$$

## §3.2.3 More on Regression (Chp 13)

### 3.2.3A Multiple linear regression

- Modeling

$$
Y=\beta_{0}+\beta_{1} X_{1}+\ldots+\beta_{K} X_{K}+\epsilon
$$

$E(\epsilon)=0, V(\epsilon)=\sigma^{2}$.
With the data from $n$ indpt units: $\left\{\left(Y_{i}, X_{1 i}, \ldots, X_{K i}\right): i=1, \ldots, n\right\}$

$$
Y_{i}=\beta_{0}+\beta_{1} X_{1 i}+\ldots+\beta_{K} X_{K i}+\epsilon_{i}
$$

$\epsilon_{i}$ indpt with $E\left(\epsilon_{i}\right)=0$ and $V\left(\epsilon_{i}\right)=\sigma^{2}$.
Alternative presentation: $\underline{Y}=\mathbf{X} \underline{\beta}+\underline{\epsilon}$ with $E(\underline{\epsilon})=\underline{0}$ and $V(\underline{\epsilon})=\operatorname{diag}\left(\sigma^{2}, \ldots, \sigma^{2}\right)$.

## Inferences with the Multiple Linear Regression Model

(a) Estm of $\beta_{0}, \ldots, \beta_{K}$ by LSE: $\hat{\beta}_{0}, \ldots, \hat{\beta}_{K}$

$$
L\left(\hat{\beta}_{0}, \ldots, \hat{\beta}_{K}\right)=\min _{\underline{\beta}} L\left(\beta_{0}, \ldots, \beta_{K}\right)
$$

with $L\left(\beta_{0}, \ldots, \beta_{K}\right)=\sum_{i=1}^{n}\left(Y_{i}-\left[\beta_{0}+\beta_{1} X_{1 i}+\ldots+\beta_{K} X_{K i}\right]\right)^{2}$.

$$
\underline{\hat{\beta}}=\left(\mathbf{X}^{\prime} \mathbf{X}\right)^{-1} \mathbf{X}^{\prime} \underline{Y}
$$

Properties of LSE:
(i) $\hat{\beta}$ is the best unbiased linear estm
(ii) If $\epsilon_{i} \sim N\left(0, \sigma^{2}\right)$ iid, $\hat{\beta}$ is the MLE and
$\underline{\hat{\beta}} \sim N\left(\underline{\beta}, \sigma^{2}\left(\mathbf{X}^{\prime} \mathbf{X}\right)^{-1}\right)$
(b) Estimation of $\sigma^{2}$ : unbiased $\hat{\sigma}^{2}=M S S_{e}$

$$
S S_{e}=\sum_{i=1}^{n} e_{i}^{2}=\sum_{i=1}^{n}\left(Y_{i}-\hat{Y}_{i}\right)^{2}
$$

with $\hat{Y}_{i}=\hat{\beta}_{0}+\hat{\beta}_{1} X_{1 i}+\ldots+\hat{\beta}_{K} X_{K i}$. Let $M S S_{e}=S S_{e} /[n-(K+1)]$.
(c) Associated ANOVA with $\epsilon_{i} \sim N\left(0, \sigma^{2}\right)$ iid

$$
S S_{T}=\sum_{i=1}^{n}\left(Y_{i}-\bar{Y}\right)^{2}, \quad S S_{e}=\sum_{i=1}^{n}\left(Y_{i}-\hat{Y}_{i}\right)^{2} \quad S S_{r e g}=S S_{T}-S S_{e}
$$

$H_{0}: \beta_{1}=\ldots=\beta_{K}=0$ vs $H_{1}$ : otherwise. [Test for Model Utility]

| Source of Variation | df | SS | F-value |
| :---: | :---: | :---: | :---: |
| regression | $K$ | $S S_{\text {reg }}$ | $F=\frac{M S S_{\text {reg }}}{M S S_{e}}$ |
| error | $n-(K+1)$ | $S S_{e}$ | $\sim F(K, n-(K+1))$ under $H_{0}$ |
| total | $n-1$ | $S S_{T}$ |  |

- Coef of determination. $R^{2}=S S_{\text {reg }} / S S_{T}=1-S S_{e} / S S_{T}$, multiple correlation coef $R$
- Adjusted $R^{2}$. $\bar{R}^{2}=1-M S S_{e} / M S S_{T}$, to adjust for num of explanatory variables in the model.
(d) Interval estimation
(i) Cl of $\beta_{k}$ with $1-\alpha$ level: $\hat{\beta}_{k} \pm t_{\alpha / 2}(n-(K+1)) s_{\hat{\beta}_{k}}$
(ii) Cl of $\mu_{Y \mid X_{1}^{*}, \ldots, X_{K}^{*}}=\beta_{0}+\beta_{1} X_{1}^{*}+\ldots+\beta_{K} X_{K}^{*}$ with $1-\alpha$ level $\hat{\mu}_{Y \mid X_{1}^{*}, \ldots, X_{\kappa}^{*}} \pm t_{\alpha / 2}(n-(K+1)) s_{\hat{\mu}_{\underline{X}^{*}}}$

Here estm $\hat{Y}_{\underline{X}^{*}}=\hat{\mu}_{\underline{X}^{*}} ; V\left(\hat{\mu}_{\underline{X}}{ }^{*}\right)=\sigma^{2} \underline{X}^{*^{\prime}}\left(\mathbf{X}^{\prime} \mathbf{X}\right)^{-1} \underline{\underline{X}}^{*}$
(iii) PI of $Y$ at $\underline{x}^{*^{\prime}}=\left(x_{1}^{*}, \ldots, x_{K}^{*}\right)$ with $1-\alpha$ level

$$
\hat{\mu}_{Y \mid X_{1}^{*}, \ldots, x_{K}^{*}} \pm t_{\alpha / 2}(n-(K+1)) \sqrt{s^{2}+s_{\hat{\mu}_{X^{*}}}^{2}}
$$

Anything really new in multiple linear regression?
$\Longrightarrow(e)$ Variable selection: to be studied soon ... ...

Example 7.2 (textbook p583)

- Study. reported by an article in J of the Amer Ceramic Soc (2012):
$Y=$ glass microhardness resulted from various compositions;

$$
X_{1}=N ; X_{2}=F
$$

- Data: $n=18$ indpt obs

$$
Y_{i}=\beta_{0}+\beta_{1} X_{1 i}+\beta_{2} X_{2 i}+\epsilon_{i}, \quad i=1, \ldots, n
$$

assuming $\epsilon_{i} \sim N\left(0, \sigma^{2}\right)$.

- the fitted model: $Y=6.23+0.0618 X_{1}-0.0387 X_{2}$
- $R^{2}=98.4 \%$
- $95 \% \mathrm{CI}$ for $\beta_{1}$ : (.0573,.0663); $95 \% \mathrm{CI}$ for $\beta_{2}:(-.0626,-.0148)$
- $95 \% \mathrm{Cl}$ for average hardness when $X_{1}=20, X_{2}=1:(7.35,7.50)$
- $95 \% \mathrm{PI}$ for an observed hardness when $X_{1}=20, X_{2}=1:(7.20$, 7.65)


## (e) Variable selection

To select from $X_{1}, \ldots, X_{K}$ the "important" (significant) explanatory variables for $Y$

- Procedures when $K \gg 1$, the exhaustive search hard to implement
- (i) Forward Selection: starting from the most important explanatory variable and gradually adding to the list the important ones
- (ii) Backward Elimination: starting from the full list and gradually eliminating the non-important variables
- (iii) Forward-Backward/Backward-Forward Selection:

Assessing "importance": various criteria
(i) $R^{2}$-value, Adjusted $R^{2}$-value;
(ii) Akaike's Information Criterion (AIC):
$-2 \ln L+2 p$ ( $L=$ maximum likelihood, closely related to Kullback-Leibler information) the smaller, the better,
(iii) Bayesian Information Criterion (BIC):
$-2 \ln L+p \ln n$ the smaller, the better.
(iv) Hypothesis testings

## What will we study next?

Part 1. Introduction and Review (Chp 1-5)
Part 2. Basic Statistical Inference (Chp 6-9)
Part 3. Important Topics in Statistics (Chp 10-13)
3.1A One-Factor Analysis of Variance (Chp 10)
3.1B Multi-Factor ANOVA (Chp 11)
3.2A Simple Linear Regression Analysis (Chp 12)
3.2B More on Regression (Chp 13)
3.2.3A Multiple linear regression
3.2.3B Regression with transformed variables
3.2.3C Categorical predictors
3.2.3D Discussion

Part 4. Further Topics (Selected from Chp 14-16)

