Model Selection
Model Diagnostics
Non-Constant Variance & Transformation

Lecture 4

Multiple Linear Regression: Model Selection and Model Checking

Reading: Faraway (2014) Chapters 6, 9.1, and 10

DSA 8020 Statistical Methods II

Whitney Huang
Clemson University

Agenda

1 Model Selection

2 Model Diagnostics

3 Non-Constant Variance & Transformation

Model Selection in Multiple Linear Regression

Multiple Linear Regression Model:

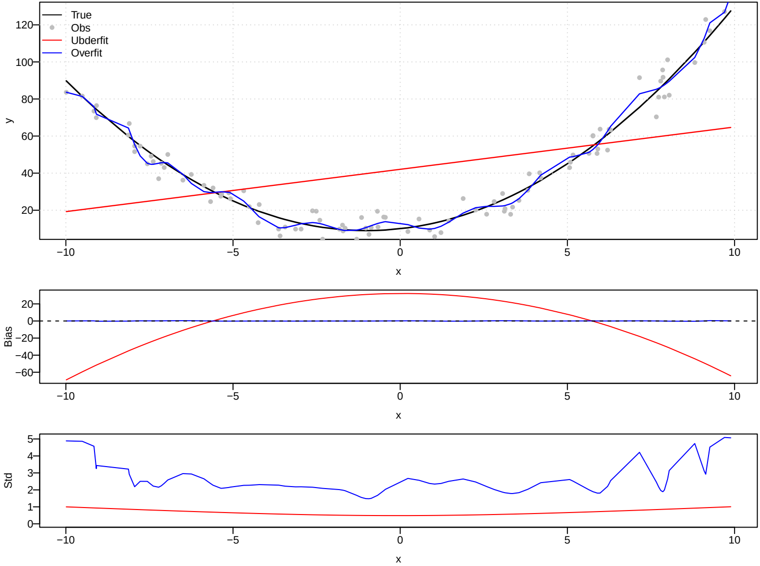
$$Y_i = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_{p-1} x_{p-1} + \varepsilon_i, \quad \varepsilon_i \overset{i.i.d.}{\sim} \mathrm{N}(0, \sigma^2)$$

Basic Problem: how to choose between competing linear regression models?

- Model too "small": underfit the data; poor predictions; high **bias**; low **variance**
- Model too big: "overfit" the data; poor predictions; low **bias**; high **variance**

In the next few slides we will discuss some commonly used model selection criteria to choose the "right" model

An Example of Bias and Variance Tradeoff



Balancing Bias And Variance: Mallows' C_p Criterion

A good model should balance **bias** and **variance** to get good predictions

$$
\begin{aligned}
(\hat{Y}_i - \mu_i)^2 &= (\hat{Y}_i - \mathrm{E}(\hat{Y}_i) + \mathrm{E}(\hat{Y}_i) - \mu_i)^2 \\
&= \underbrace{(\hat{Y}_i - \mathrm{E}(\hat{Y}_i))^2}_{\sigma^2_{\hat{Y}_i} \text{ Variance}} + \underbrace{(\mathrm{E}(\hat{Y}_i) - \mu_i)^2}_{\text{Bias}^2},
\end{aligned}
$$

where $\mu_i = \mathrm{E}(Y_i | X_i = x_i)$

- Mean squared prediction error (MSPE): $\sum_{i=1}^n \sigma^2_{\hat{Y}_i} + \sum_{i=1}^n (\mathrm{E}(\hat{Y}_i) - \mu_i)^2$
- C_p criterion measure:

$$
\begin{aligned}
\Gamma_p &= \frac{\sum_{i=1}^n \sigma^2_{\hat{Y}_i} + \sum_{i=1}^n (\mathrm{E}(\hat{Y}_i) - \mu_i)^2}{\sigma^2} \\
&= \frac{\sum \text{Var}_{\text{pred}} + \sum \text{Bias}^2}{\text{Var}_{\text{error}}}
\end{aligned}
$$

C_p Criterion

C_p statistic:

$$C_p = \frac{\text{SSE}}{\text{MSE}_\text{F}} + 2p - n$$

- When model is correct $\mathrm{E}(C_p) \approx p$
- When plotting models against p
  - Biased models will fall above $C_p = p$
  - Unbiased models will fall around line $C_p = p$
  - By definition: C_p for full model equals p

We desire models with small p and C_p around or less than p. See R session for an example

Adjusted R^2 Criterion

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Adjusted R^2, denoted by R^2_{adj}, attempts to take account of the phenomenon of the R^2 automatically and spuriously increasing when extra explanatory variables are added to the model.

$$R^2_{\text{adj}} = 1 - \frac{\text{SSE}/(n-p-1)}{\text{SST}/(n-1)}$$

- Choose model which maximizes R^2_{adj}
- Same approach as choosing model with smallest MSE

Predicted Residual Sum of Squares $PRESS$ Criterion

- For each observation i, predict Y_i using model generated from other $n-1$ observations
- Use $PRESS = \sum_{i=1}^{n}(Y_i - \hat{Y}_{i(i)})^2$ to quantify the out-of-sample prediction performance
- Want to select model with smallest $PRESS$
- $PRESS$ statistic is a form of cross-validation

Information criteria

There are two widely used information criteria:

- Akaike's information criterion (AIC)

$$n\log(\frac{\mathsf{SSE}_k}{n}) + 2k$$

- Bayesian information criterion (BIC)

$$n\log(\frac{\mathsf{SSE}_k}{n}) + k\log(n)$$

Here k is the number of the parameters in the model.

Automatic Search Procedures

- Forward Selection: begins with no predictors and then adds in predictors one by one using some criterion (e.g., p-value or AIC)
- Backward Elimination: starts with all the predictors and then removes predictors one by one using some criterion
- Stepwise Search: a combination of backward elimination and forward selection. Can add or delete predictor at each stage
- All Subset Selection: Comparing all possible models using a selected criterion. Impractical for “large” number of predictors

Model Assumptions

Model:

$$Y_i = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_{p-1} x_{p-1} + \varepsilon_i, \quad \varepsilon_i \overset{i.i.d.}{\sim} \mathrm{N}(0, \sigma^2)$$

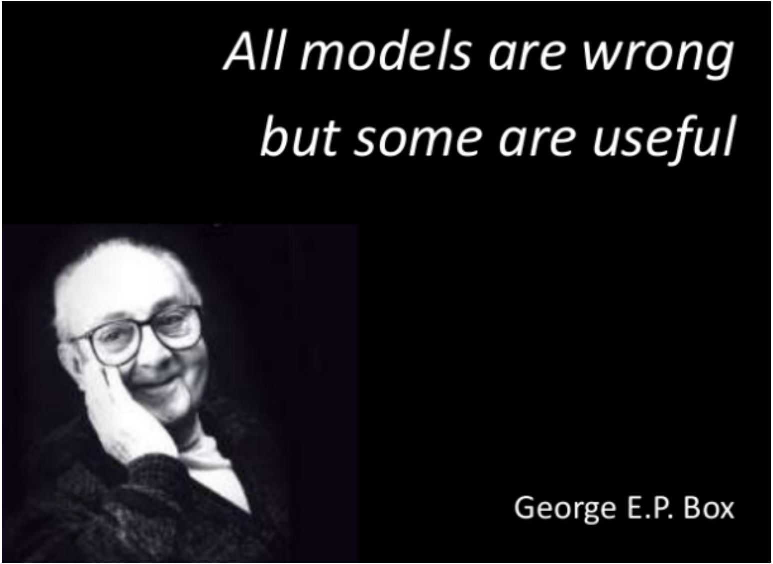
We make the following assumptions:

- Linearity:

$$\mathrm{E}(Y | x_1, x_2, \cdots, x_{p-1}) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_{p-1} x_{p-1}$$

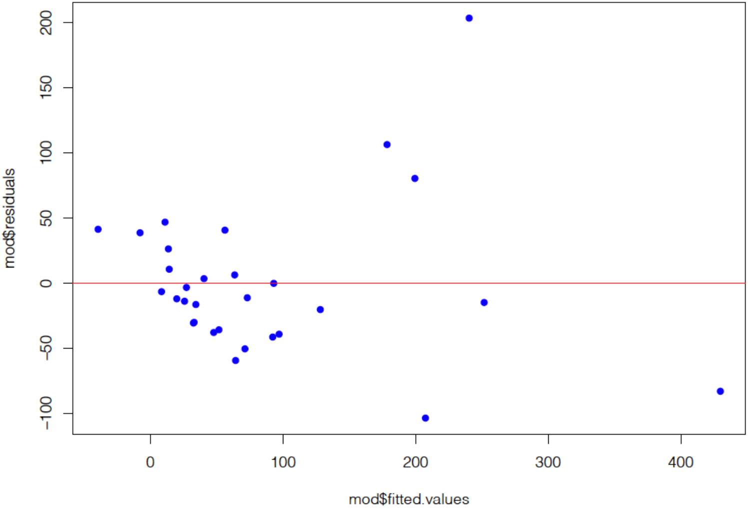
- Errors have constant variance, are independent, and normally distributed

$$\varepsilon_i \overset{i.i.d.}{\sim} \mathrm{N}(0, \sigma^2)$$


All models are wrong
but some are useful
George E.P. Box

Residuals versus Fits Plot

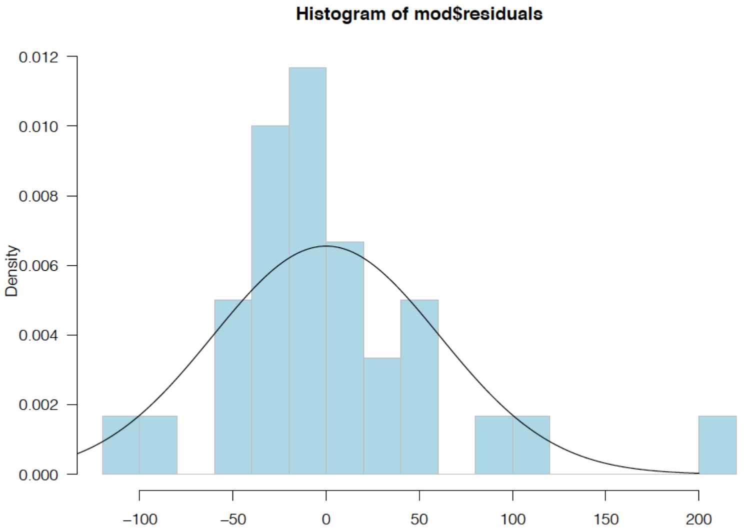
```
plot(mod$fitted.values, mod$residuals, pch = 16, col = "blue")
abline(h = 0, col = "red")
```



We will revisit this in the end of the lecture

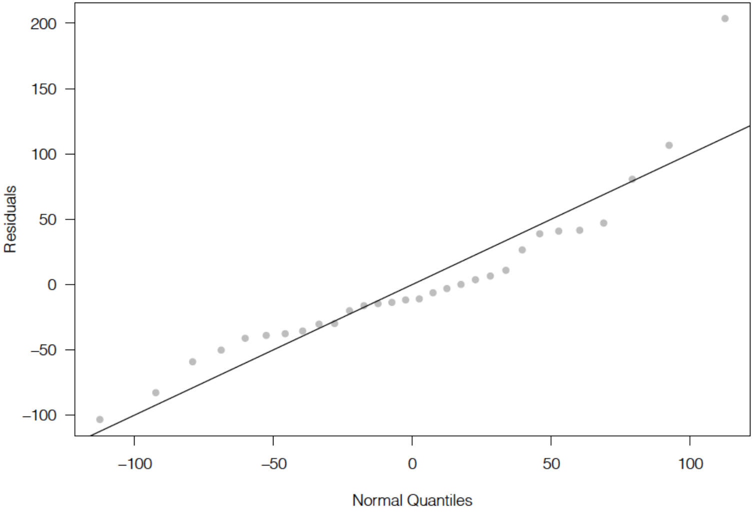
Assessing Normality of Residuals: Histogram

```
par(las = 1)
hist(mod$residuals, 12, prob = T,
     col = "lightblue", border = "gray")
xg <- seq(-200, 200, 1)
yg <- dnorm(xg, 0, 60.86)
lines(xg, yg)
```



Assessing Normality of Residuals: QQ Plot

```
plot(qnorm(1:30 / 31, 0, 60.86), sort(mod$residuals), pch = 16,
     col = "gray", xlab = "Normal Quantiles", ylab = "Residuals")
abline(0, 1)
```



Leverage: Detecting "Extreme" Predictor Values

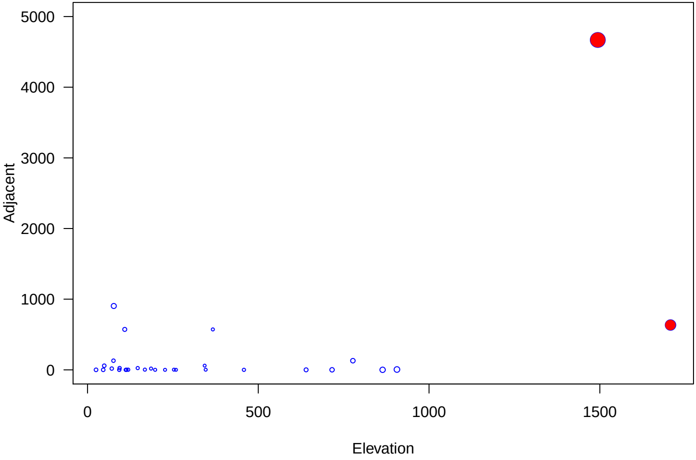
Recall in MLR that $\hat{y} = \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y} = \boldsymbol{H}\boldsymbol{y}$ where $\boldsymbol{H}$ is the hat-matrix

- The leverage value for the i_{th} observation is defined as:

$$h_i = \boldsymbol{H}_{ii}$$

- Can show that Var$(e_i) = \sigma^2(1 - h_i)$, where $e_i = y_i - \hat{y}_i$ is the residual for the i_{th} observation
- $\frac{1}{n} \leq h_i \leq 1, \quad 1 \leq i \leq n$ and $\bar{h} = \sum_{i=1}^{n} \frac{h_i}{n} = \frac{p}{n} \Rightarrow$ a "rule of thumb" is that leverages of more than $\frac{2p}{n}$ should be looked at more closely

Leverage Values of `Species` $\sim$ `Elev` $+$ `Adj`



Studentized Residuals

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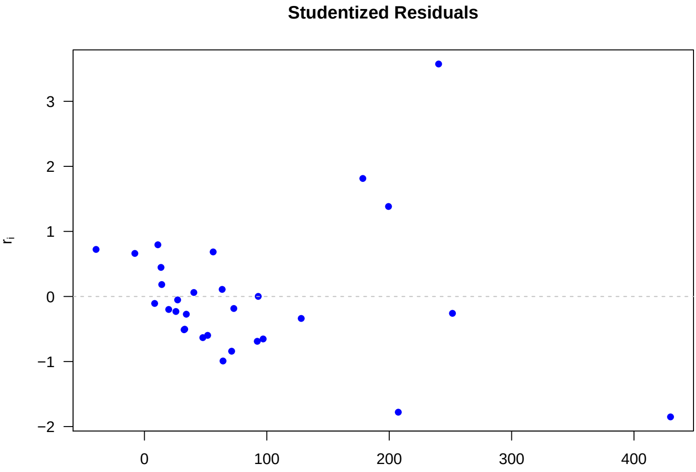
As we have seen Var$(e_i) = \sigma^2(1 - h_i)$, this suggests the use of $r_i = \frac{e_i}{\hat{\sigma}\sqrt{(1-h_i)}}$

- r_i's are called **studentized residuals**. r_i's are sometimes preferred in residual plots as they have been standardized to have equal variance.
- If the model assumptions are correct then Var$(r_i) = 1$ and Corr(r_i, r_j) tends to be small

Studentized Residuals of `Species` ~ `Elev` + `Adj`



Studentized Deleted Residuals

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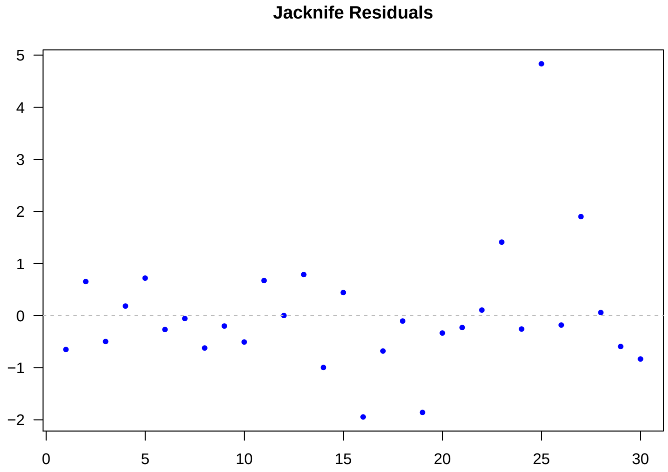
- For a given model, exclude the observation i and recompute $\hat{\boldsymbol{\beta}}_{(i)}$, $\hat{\sigma}_{(i)}$ to obtain $\hat{y}_{i(i)}$
- The observation i is an outlier if $\hat{y}_{i(i)} - y_i$ is "large"
- Can show
  $\text{Var}(\hat{y}_{i(i)} - y_i) = \sigma^2_{(i)}\left(1 + \boldsymbol{x}_i^T(\boldsymbol{X}^T_{(i)}\boldsymbol{X}_{(i)})^{-1}\boldsymbol{x}_i\right) = \frac{\sigma^2_{(i)}}{1-h_i}$
- Define the **Studentized Deleted Residuals** as

$$t_i = \frac{\hat{y}_{i(i)} - y_i}{\sqrt{\hat{\sigma}^2_{(i)}(1-h_i)}} = \frac{\hat{y}_{i(i)} - y_i}{\sqrt{\text{MSE}_{(i)}(1-h_i)^{-1}}}$$

which are distributed as a t_{n-p-1} if the model is correct and $\varepsilon \sim \text{N}(\boldsymbol{0}, \sigma^2\boldsymbol{I})$

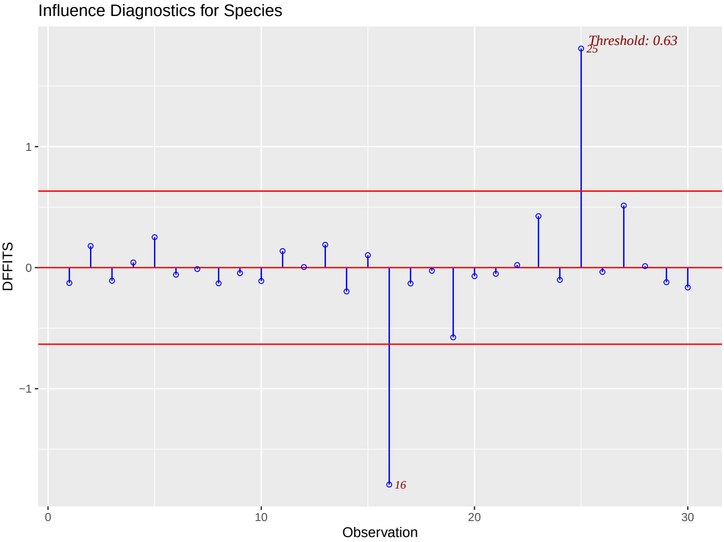
Jackknife Residuals of `Species` ~ `Elev` + `Adj`



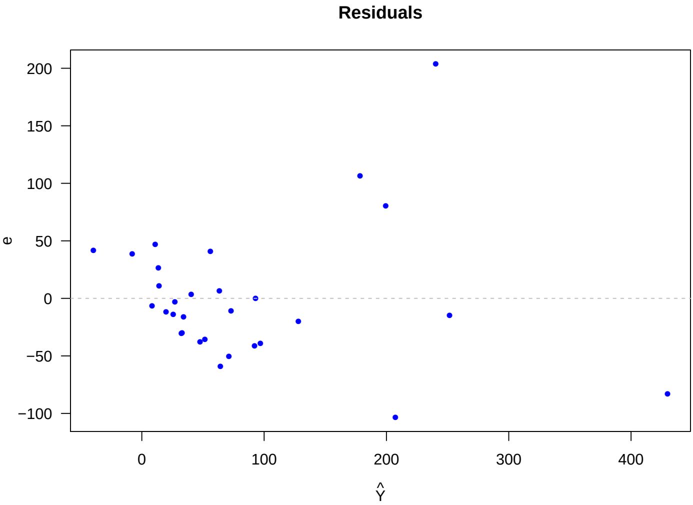
DFFITS

- Difference between the fitted values $\hat{y}_i$ and the predicted values $\hat{y}_{i(i)}$
- $\text{DFFITS}_i = \frac{\hat{y}_i - \hat{y}_{i(i)}}{\sqrt{\text{MSE}_{(i)} h_i}}$
- Concern if absolute value greater than 1 for small data sets, or greater than $2\sqrt{p/n}$ for large data sets

DFFITS of `Species` ~ `Elev` + `Adj`

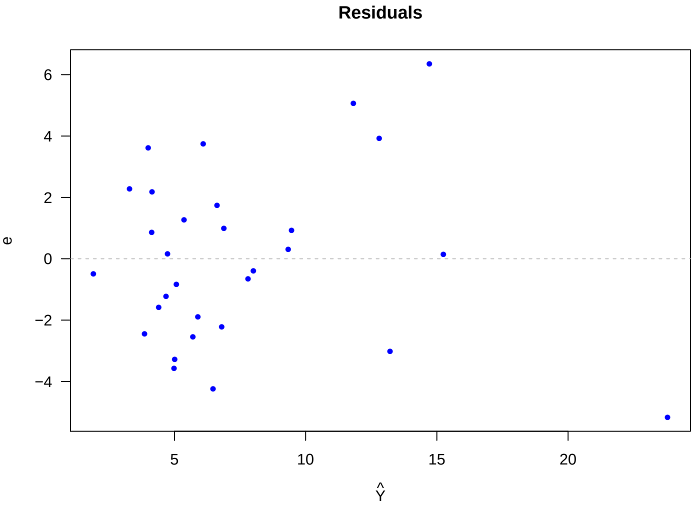


Residual Plot of `Species` ~ `Elev` + `Adj`



Residual Plot After Square Root Transformation

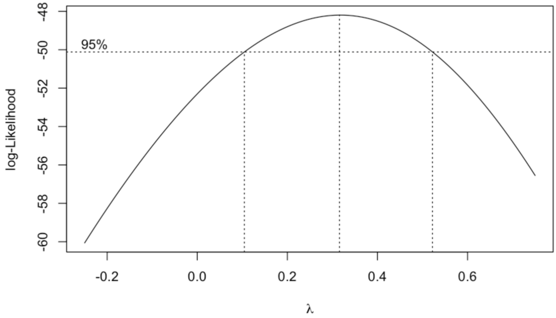
$$\sqrt{\text{Species}} \sim \text{Elev} + \text{Adj}$$



Box-Cox Transformation

The Box-Cox method [Box and Cox, 1964] is a powerful way to determine if a transformation on the response is needed

$$g_\lambda(y) = \begin{cases} \frac{y^\lambda - 1}{\lambda} & \text{if } \lambda \neq 0; \\ \log(y) & \text{if } \lambda = 0. \end{cases}$$



In `R`, we can use the `boxcox` function from the `MASS` package to perform a Box-Cox transformation. The plot suggests a cube root may be needed

Summary

Model Selection
Model Diagnostics
Non-Constant Variance & Transformation

This slides cover:

- Model/variable selection can be done via some criterion-based methods to balance bias and variance
- Model diagnostics is crucial to ensure valid statistical inference
- Box-Cox Transformation can be used to transform the response in order to correct model violations