Lecture 4

Multiple Linear Regression II

Reading: Forecasting, Time Series, and Regression (4th edition) by Bowerman, O'Connell, and Koehler: Chapter 4

MATH 4070: Regression and Time-Series Analysis

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Agenda

1. General Linear F-Test
2. Prediction
3. Multicollinearity
4. Model Selection
5. Model Diagnostics
6. Non-Constant Variance & Transformation

Review: t-Test and F-Test in Linear Regression

- t-test: Testing one predictor
  1. **Null/Alternative Hypotheses**: $H_0 : \beta_j = 0$ vs. $H_a : \beta_j \neq 0$
  2. **Test Statistic**: $t^* = \frac{\hat{\beta}_j - 0}{\hat{\text{se}}(\hat{\beta}_j)}$
  3. Reject H_0 if $|t^*| > t_{1-\alpha/2, n-p}$
- Overall F-test: Test of all the predictors
  1. $H_0 : \beta_1 = \beta_2 = \cdots = \beta_{p-1} = 0$
  2. $H_a :$ at least one $\beta_j \neq 0, 1 \leq j \leq p-1$
  3. **Test Statistic**: $F^* = \frac{\text{MSR}}{\text{MSE}}$
  4. Reject H_0 if $F^* > F_{1-\alpha, p-1, n-p}$

Both tests are special cases of General Linear F-test

General Linear F-Test

- Comparison of a "full model" and "reduced model" that involves **a subset of full model predictors**
- Consider a full model with k predictors and reduced model with ℓ predictors ($\ell < k$)
- Test statistic: $F^* = \frac{(\text{SSE}_{\text{reduce}} - \text{SSE}_{\text{full}})/(k-\ell)}{\text{SSE}_{\text{full}}/(n-k-1)}$ $\Rightarrow$ Testing H_0 that the regression coefficients for the extra variables are all zero
  - Example 1: $x_1, x_2, \cdots, x_{p-1}$ vs. intercept only $\Rightarrow$ Overall F-test

General Linear F-Test

- Comparison of a “full model” and “reduced model” that involves **a subset of full model predictors**

- Consider a full model with k predictors and reduced model with ℓ predictors ($\ell < k$)

- Test statistic: $F^* = \frac{(\text{SSE}_{\text{reduce}} - \text{SSE}_{\text{full}})/(k-\ell)}{\text{SSE}_{\text{full}}/(n-k-1)}$ $\Rightarrow$ Testing H_0 that the regression coefficients for the extra variables are all zero

    - Example 1: $x_1, x_2, \cdots, x_{p-1}$ vs. intercept only $\Rightarrow$ Overall F-test

    - Example 2: $x_j, 1 \le j \le p-1$ vs. intercept only $\Rightarrow$ t-test for β_j

General Linear F-Test

- Comparison of a “full model” and “reduced model” that involves **a subset of full model predictors**

- Consider a full model with k predictors and reduced model with ℓ predictors ($\ell < k$)

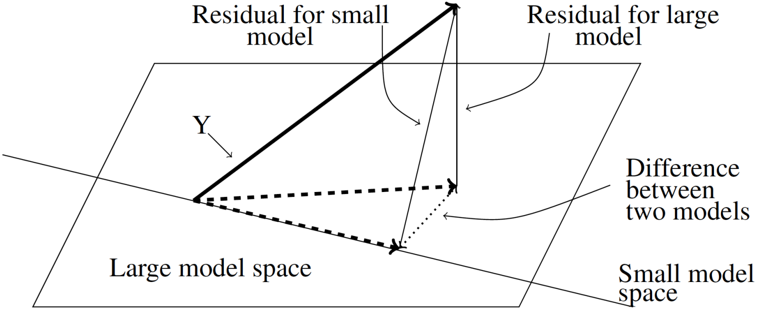
- Test statistic: $F^* = \frac{(\text{SSE}_{\text{reduce}} - \text{SSE}_{\text{full}})/(k-\ell)}{\text{SSE}_{\text{full}}/(n-k-1)}$ ⇒ Testing H_0 that the regression coefficients for the extra variables are all zero

  - Example 1: $x_1, x_2, \cdots, x_{p-1}$ vs. intercept only ⇒ Overall F-test

  - Example 2: $x_j, 1 \le j \le p-1$ vs. intercept only ⇒ t-test for β_j

  - Example 3: x_1, x_2, x_3, x_4 vs. x_1, x_3 ⇒ $H_0 : \beta_2 = \beta_4 = 0$

Geometric Illustration of General Linear F-Test



Source: Faraway, *Linear Models with* R, 2014, p.34

Species Diversity on the Galapagos Islands: Full Model

```
> summary(gala_fit2)

Call:
lm(formula = Species ~ Elevation + Area)

Residuals:
     Min       1Q   Median       3Q      Max 
-192.619  -33.534  -19.199    7.541  261.514 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)   
(Intercept) 17.10519   20.94211   0.817  0.42120   
Elevation    0.17174    0.05317   3.230  0.00325 **
Area         0.01880    0.02594   0.725  0.47478   
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 79.34 on 27 degrees of freedom
Multiple R-squared:  0.554,	Adjusted R-squared:  0.521 
F-statistic: 16.77 on 2 and 27 DF,  p-value: 1.843e-05
```

Species Diversity on the Galapagos Islands: Reduce Model


```
> summary(gala_fit1)

Call:
lm(formula = Species ~ Elevation)

Residuals:
     Min       1Q   Median       3Q      Max 
-218.319  -30.721  -14.690    4.634  259.180 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept) 11.33511   19.20529   0.590     0.56    
Elevation    0.20079    0.03465   5.795 3.18e-06 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 78.66 on 28 degrees of freedom
Multiple R-squared:  0.5454,    Adjusted R-squared:  0.5291 
F-statistic: 33.59 on 1 and 28 DF,  p-value: 3.177e-06
```

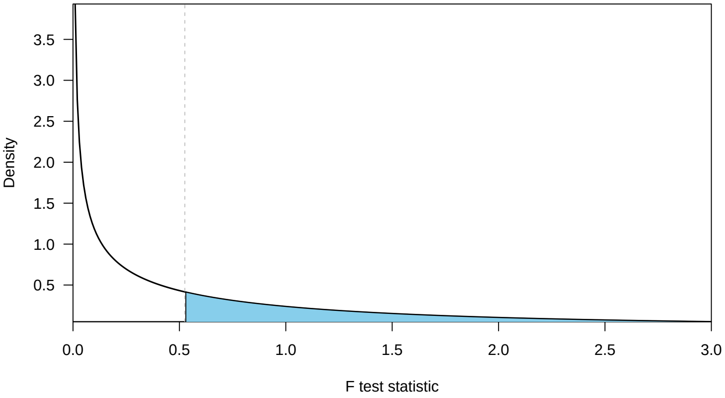
Performing a General Linear F-Test

- $H_0 : \beta_{\texttt{Area}} = 0$ vs. $H_a : \beta_{\texttt{Area}} \neq 0$
- $F^* = \dfrac{(173254-169947)/(2-1)}{169947/(30-2-1)} = 0.5254$
- p-value: $\mathbb{P}[F > 0.5254] = 0.4748$, where $F \sim \mathrm{F}_{\underbrace{1}_{k-\ell},\ \underbrace{27}_{n-k-1}}$

```
> anova(gala_fit1, gala_fit2)
Analysis of Variance Table

Model 1: Species ~ Elevation
Model 2: Species ~ Elevation + Area
  Res.Df    RSS Df Sum of Sq      F Pr(>F)
1     28 173254
2     27 169947  1      3307 0.5254 0.4748
```

Visualizing p-value



p-value is the shaped area under the density curve of the null distribution

Another Example of General Linear F-Test

```
> full <- lm(Species ~ Area + Elevation + Nearest + Scruz + Adjacent,
 data = gala)
> anova(full)
Analysis of Variance Table

Response: Species
          Df Sum Sq Mean Sq F value    Pr(>F)
Area       1 145470  145470 39.1262 1.826e-06 ***
Elevation  1  65664   65664 17.6613 0.0003155 ***
Nearest    1     29      29  0.0079 0.9300674
Scruz      1  14280   14280  3.8408 0.0617324 .
Adjacent   1  66406   66406 17.8609 0.0002971 ***
Residuals 24  89231    3718
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
> reduced <- lm(Species ~ Elevation + Adjacent)
> anova(reduced)
Analysis of Variance Table

Response: Species
          Df Sum Sq Mean Sq F value    Pr(>F)
Elevation  1 207828  207828  56.112 4.662e-08 ***
Adjacent   1  73251   73251  19.777 0.0001344 ***
Residuals 27 100003    3704
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Performing a General Linear F-Test

- Null and alternative hypotheses:

$$H_0 : \beta_{\texttt{Area}} = \beta_{\texttt{Nearest}} = \beta_{\texttt{Scruz}} = 0$$
$$H_a : \text{ at least one of the three coefficients} \neq 0$$

- $F^* = \dfrac{(100003-89231)/(5-2)}{89231/(30-5-1)} = 0.9657$

- p-value: $\mathbb{P}[F > 0.9657] = 0.425$, where $F \sim \mathrm{F}_{3,24}$

```
> anova(reduced, full)
Analysis of Variance Table

Model 1: Species ~ Elevation + Adjacent
Model 2: Species ~ Area + Elevation + Nearest + Scruz + Adjacent
  Res.Df    RSS Df Sum of Sq      F Pr(>F)
1     27 100003
2     24  89231  3     10772 0.9657  0.425
```

Multiple Linear Regression Prediction

Given a new set of predictors, $\boldsymbol{x}_0 = (1, x_{0,1}, x_{0,2}, \cdots, x_{0,p-1})^{\mathrm{T}}$, the predicted response is

$$\hat{y}_0 = \hat{\beta}_0 + \hat{\beta}_1 x_{0,1} + \hat{\beta}_2 x_{0,2} + \cdots + \hat{\beta}_{p-1} x_{0,p-1}.$$

Again, we can use matrix representation to simplify the notation

$$\hat{y}_0 = \boldsymbol{x}_0^{\mathrm{T}} \hat{\boldsymbol{\beta}},$$

where $\boldsymbol{x}_0^{\mathrm{T}} = (1, x_{0,1}, x_{0,2}, \cdots, x_{0,p-1})$

We will use this formula to carry out two different kinds of predictions

Two Kinds of Predictions

There are two kinds of predictions can be made for a given $\boldsymbol{x}_0$:

- **Predicting a future response:**

  Based on MLR, we have $y_0 = \boldsymbol{x}_0^{\mathrm{T}}\boldsymbol{\beta} + \varepsilon$. Since $E(\varepsilon) = 0$, therefore the predicted value is

$$\hat{y}_0 = \boldsymbol{x}_0^{\mathrm{T}}\hat{\boldsymbol{\beta}}$$

- **Predicting the mean response:**

  Since $E(y_0) = \boldsymbol{x}_0^{\mathrm{T}}\boldsymbol{\beta}$, there we have the predicted mean response

$$\widehat{E(y_0)} = \boldsymbol{x}_0^{\mathrm{T}}\hat{\boldsymbol{\beta}},$$

  the same predicted value as predicting a future response

Next, we need to assess their prediction uncertainties, and then we will identify the differences in terms of these uncertainties

Prediction Uncertainty

From page 30 of slides 3, we have $\mathrm{Var}(\hat{\boldsymbol{\beta}}) = \sigma^2 \left(\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}\right)^{-1}$. Therefore we have

$$\mathrm{Var}(\hat{y}_0) = \mathrm{Var}(\boldsymbol{x}_0^{\mathrm{T}}\hat{\boldsymbol{\beta}}) = \sigma^2 \boldsymbol{x}_0^{\mathrm{T}} \left(\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}\right)^{-1} \boldsymbol{x}_0$$

We can now construct $100(1-\alpha)\%$ CI for the two kinds of predictions:

- **Predicting a future response y_0:**

$$\boldsymbol{x}_0^{\mathrm{T}}\hat{\boldsymbol{\beta}} \pm t_{1-\alpha/2,n-p} \times \hat{\sigma}\sqrt{\underbrace{1}_{\text{accounting for } \varepsilon} + \boldsymbol{x}_0^{\mathrm{T}} \left(\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}\right)^{-1} \boldsymbol{x}_0}$$

- **Predicting the mean response $E(y_0)$:**

$$\boldsymbol{x}_0^{\mathrm{T}}\hat{\boldsymbol{\beta}} \pm t_{1-\alpha/2,n-p} \times \hat{\sigma}\sqrt{\boldsymbol{x}_0^{\mathrm{T}} \left(\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}\right)^{-1} \boldsymbol{x}_0}$$

Example: Predicting Body Fat (Faraway 2014 Chapter 4.2)

```
lm(formula = brozek ~ age + weight + height + neck + chest +
    abdom + hip + thigh + knee + ankle + biceps + forearm + wrist,
    data = fat)

Residuals:
    Min      1Q  Median      3Q     Max
-10.264  -2.572  -0.097   2.898   9.327

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) -15.29255   16.06992  -0.952  0.34225
age           0.05679    0.02996   1.895  0.05929 .
weight       -0.08031    0.04958  -1.620  0.10660
height       -0.06460    0.08893  -0.726  0.46830
neck         -0.43754    0.21533  -2.032  0.04327 *
chest        -0.02360    0.09184  -0.257  0.79740
abdom         0.88543    0.08008  11.057  < 2e-16 ***
hip          -0.19842    0.13516  -1.468  0.14341
thigh         0.23190    0.13372   1.734  0.08418 .
knee         -0.01168    0.22414  -0.052  0.95850
ankle         0.16354    0.20514   0.797  0.42614
biceps        0.15280    0.15851   0.964  0.33605
forearm       0.43049    0.18445   2.334  0.02044 *
wrist        -1.47654    0.49552  -2.980  0.00318 **
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 3.988 on 238 degrees of freedom
Multiple R-squared:  0.749,     Adjusted R-squared:  0.7353
F-statistic: 54.63 on 13 and 238 DF,  p-value: < 2.2e-16
```

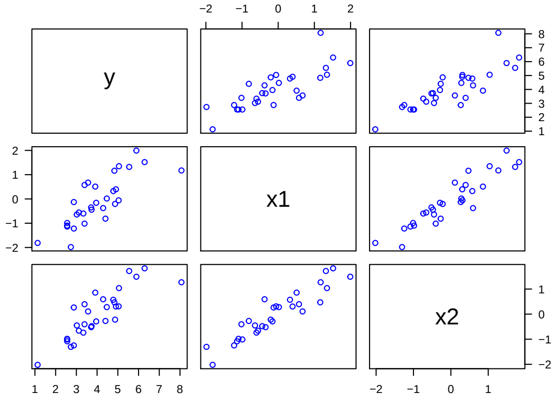
What is our prediction for the future response of a “typical” (e.g., each predictor takes its median value) man?

Example: Predicting Body Fat Cont'd

1. Calculate the median for each predictor to get $\boldsymbol{x}_0$
2. Compute the predicted value $\hat{y}_0 = \boldsymbol{x}_0^{\mathrm{T}}\hat{\boldsymbol{\beta}}$
3. Quantify the prediction uncertainty

```
> X <- model.matrix(lmod)
> (x0 <- apply(x, 2, median))
(Intercept)        age     weight     height       neck      chest      abdom
       1.00      43.00     176.50      70.00      38.00      99.65      90.95
        hip      thigh       knee      ankle     biceps    forearm      wrist
      99.30      59.00      38.50      22.80      32.05      28.70      18.30
> (y0 <- sum(x0 * coef(lmod)))
[1] 17.49322
> predict(lmod, new = data.frame(t(x0)))
       1
17.49322
> predict(lmod, new = data.frame(t(x0)), interval = "prediction")
       fit     lwr      upr
1 17.49322 9.61783 25.36861
> predict(lmod, new = data.frame(t(x0)), interval = "confidence")
       fit      lwr      upr
1 17.49322 16.94426 18.04219
```

Multicollinearity




```
> cor(sim1)
           y        x1        x2
y  1.0000000 0.7987777 0.8481084
x1 0.7987777 1.0000000 0.9281514
x2 0.8481084 0.9281514 1.0000000
```

Multicollinearity Cont'd

Multicollinearity is a phenomenon of high inter-correlations among the predictor variables

- Numerical issue ⇒ the matrix $\boldsymbol{X}^T\boldsymbol{X}$ is nearly singular
- Statistical issues/consequences
  - β's are not well estimated ⇒ spurious regression coefficient estimates
  - R^2 and predicted values are usually okay even with multicollinearity

An Simulated Example

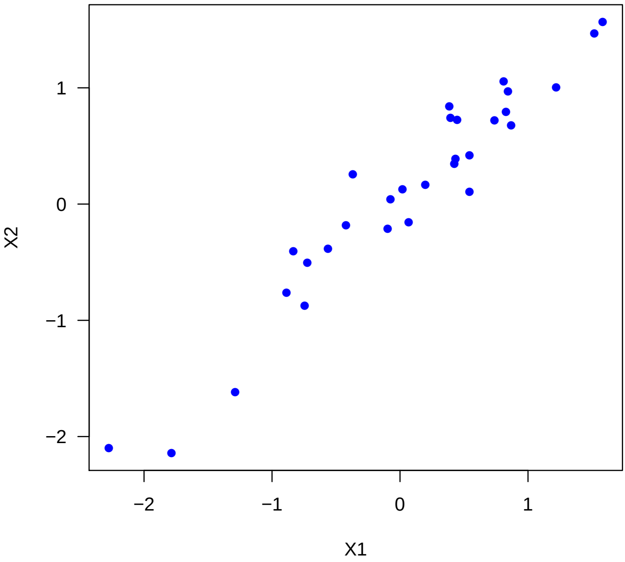
Suppose the true relationship between response y and predictors (x_1, x_2) is

$$Y = 4 + 0.8x_1 + 0.6x_2 + \varepsilon,$$

where $\varepsilon \sim \mathrm{N}(0, 1)$ and x_1 and x_2 are positively correlated with $\rho = 0.9$. Let's fit the following models:

- Model 1: $Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon_1$
  This is the true model with parameters unknown
- Model 2: $Y = \beta_0 + \beta_1 x_1 + \varepsilon_2$
  This is the wrong model because x_2 is omitted

Scatter Plot: x_1 vs. x_2



Model 1 Fit

```
Call:
lm(formula = Y ~ X1 + X2)

Residuals:
     Min       1Q   Median       3Q      Max
-1.91369 -0.73658  0.05475  0.87080  1.55150

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   4.0710     0.1778  22.898  < 2e-16 ***
X1            2.2429     0.7187   3.121  0.00426 **
X2           -0.8339     0.7093  -1.176  0.24997
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.9569 on 27 degrees of freedom
Multiple R-squared:  0.673,     Adjusted R-squared:  0.6488
F-statistic: 27.78 on 2 and 27 DF,  p-value: 2.798e-07
```

Model 2 Fit

```
Call:
lm(formula = Y ~ X1)

Residuals:
     Min       1Q   Median       3Q      Max 
-2.09663 -0.67031 -0.07229  0.87881  1.49739 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)   4.0347     0.1763  22.888  < 2e-16 ***
X1            1.4293     0.1955   7.311 5.84e-08 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.9634 on 28 degrees of freedom
Multiple R-squared:  0.6562,	Adjusted R-squared:  0.644 
F-statistic: 53.45 on 1 and 28 DF,  p-value: 5.839e-08
```

Takeaways

Model 1 fit:

```
Call:
lm(formula = Y ~ X1 + X2)

Residuals:
     Min       1Q   Median       3Q      Max 
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Coefficients:
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(Intercept)   4.0710     0.1778  22.898  < 2e-16 ***
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Model 2 fit:

```
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Coefficients:
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---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.9634 on 28 degrees of freedom
Multiple R-squared:  0.6562,	Adjusted R-squared:  0.644 
F-statistic: 53.45 on 1 and 28 DF,  p-value: 5.839e-08
```

Recall the true model:

$$Y = 4 + 0.8x_1 + 0.6x_2 + \varepsilon,$$

where $\varepsilon \sim \mathrm{N}(0,1)$, x_1 and x_2 are positively correlated with $\rho = 0.9$

Summary:

- β's are not well estimated in model 1 $\Rightarrow$ Spurious regression coefficient estimates
- In model 2, R^2 and predicted values are OK compared to model 1

Variance Inflation Factor (VIF)

We can use the variance inflation factor (VIF)

$$\text{VIF}_i = \frac{1}{1 - \text{R}_i^2}$$

to quantifies the severity of multicollinearity in MLR, where R_i^2 is the **coefficient of determination** when X_i is regressed on the remaining predictors

R example code

```
> library(faraway)
> vif(sim1[, 2:3])
      x1       x2
7.218394 7.218394
```

$\sqrt{\text{VIF}}$ indicates how much larger the standard error increases compared to if that variable had 0 correlation to other predictor variables in the model.

Model Selection in Multiple Linear Regression

Multiple Linear Regression Model:

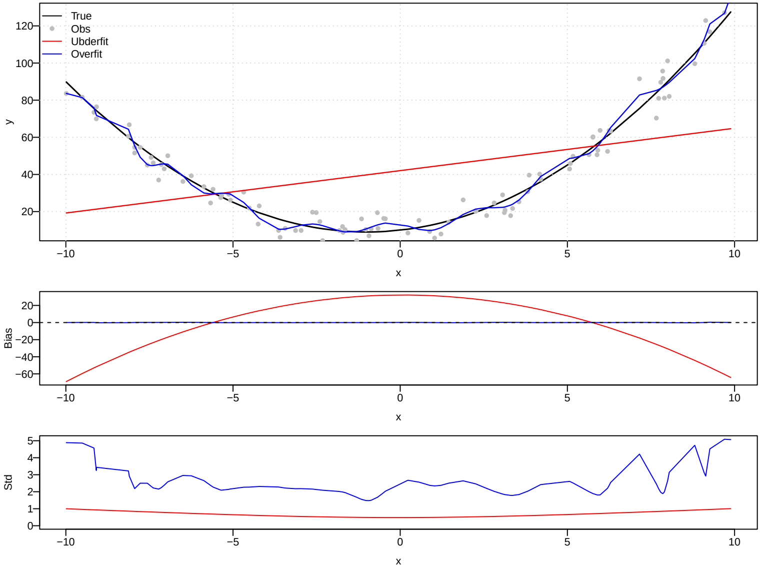
$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_{p-1} x_{p-1} + \varepsilon, \quad \varepsilon \overset{i.i.d.}{\sim} \mathrm{N}(0, \sigma^2)$$

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 to balance bias and variance

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

$$(\hat{Y}_i - \mu_i)^2 = (\hat{Y}_i - \mathbb{E}(\hat{Y}_i) + \mathbb{E}(\hat{Y}_i) - \mu_i)^2$$
$$= \underbrace{(\hat{Y}_i - \mathbb{E}(\hat{Y}_i))^2}_{\sigma^2_{\hat{Y}_i} \text{ Variance}} + \underbrace{(\mathbb{E}(\hat{Y}_i) - \mu_i)^2}_{\text{Bias}^2},$$

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

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

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

C_p Criterion

C_p statistic:

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

- When model is correct $\text{E}(C_p) \approx p$
- 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

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

Information criteria

Information criteria are statistical measures used for model selection. Commonly used information criteria include:

- Akaike's information criterion (AIC)

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

- Bayesian information criterion (BIC)

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

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

These criteria balance the goodness of fit of a model with its complexity

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:

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

We make the following assumptions:

- Linearity:

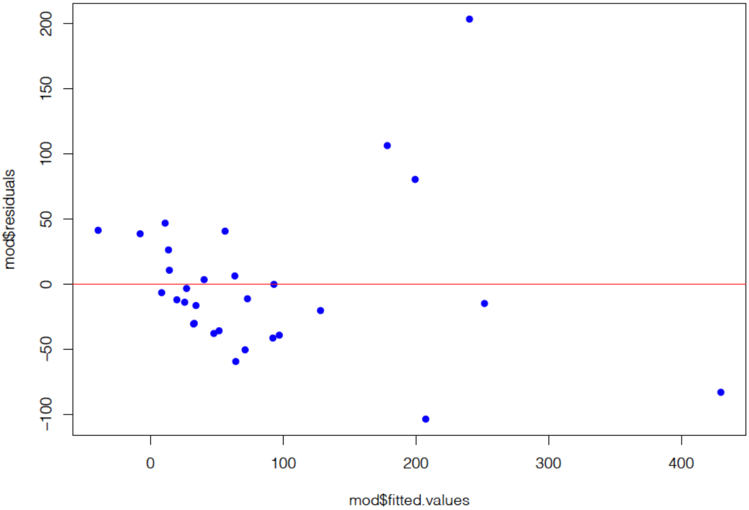
$$\mathrm{E}(Y|x_1, x_2, \cdots, x_{p-1}) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_{p-1} x_{p-1}$$

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

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

Residuals versus Fits Plot

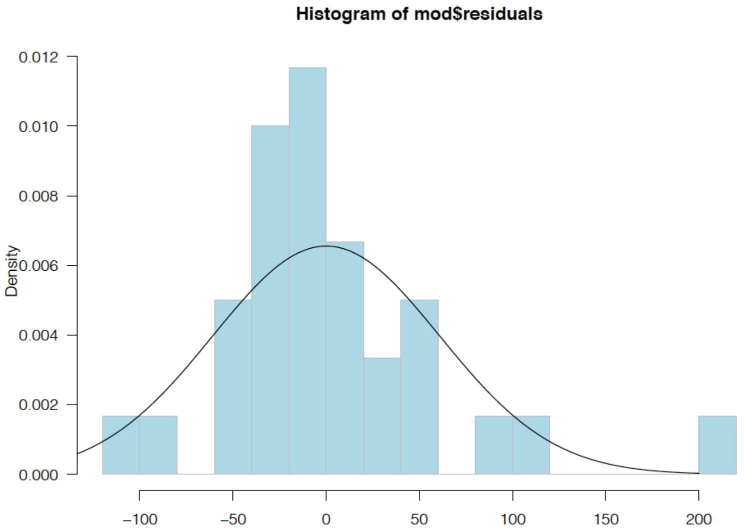
```
plot(mod$fitted.values, mod$residuals, pch = 16, col = "blue")
abline(h = 0, col = "red")
```



We will revisit this in the end of the lecture

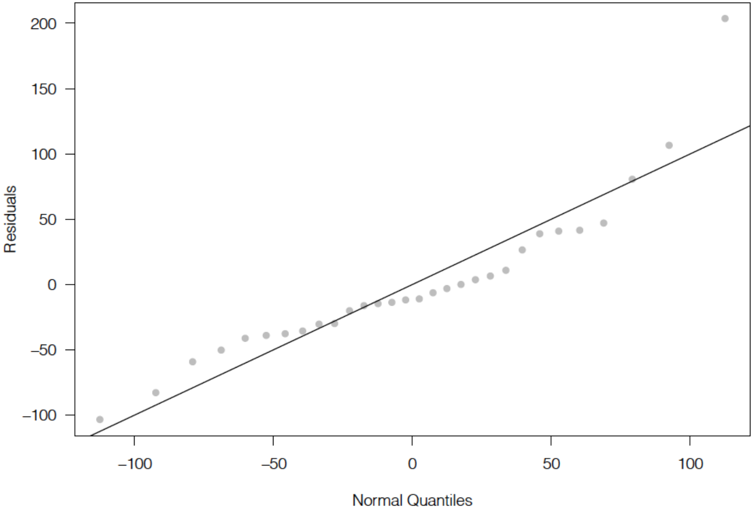
Assessing Normality of Residuals: Histogram

```
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

```r
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

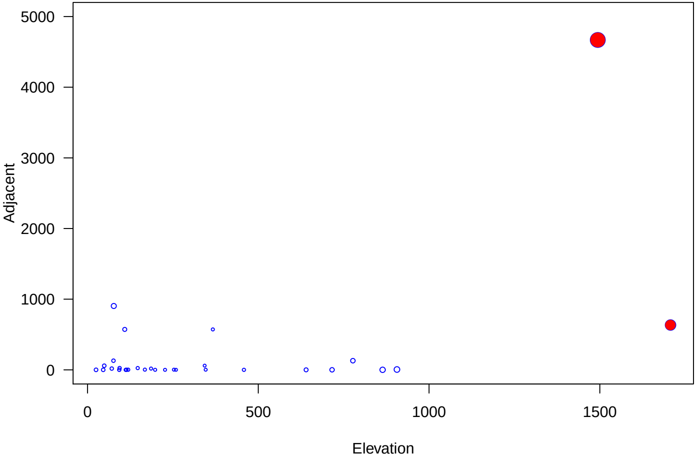
Recall in MLR that $\hat{y} = \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y} = \boldsymbol{H}\boldsymbol{y}$ where $\boldsymbol{H}$ is the hat-matrix

- 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
- $\frac{1}{n} \le h_i \le 1, \quad 1 \le i \le n$ and $\bar{h} = \sum_{i=1}^{n} \frac{h_i}{n} = \frac{p}{n} \Rightarrow$ a "rule of thumb" is that leverages greater than $\frac{2p}{n}$ should be examined more closely

Leverage Values of `Species` ~ `Elev` + `Adj`

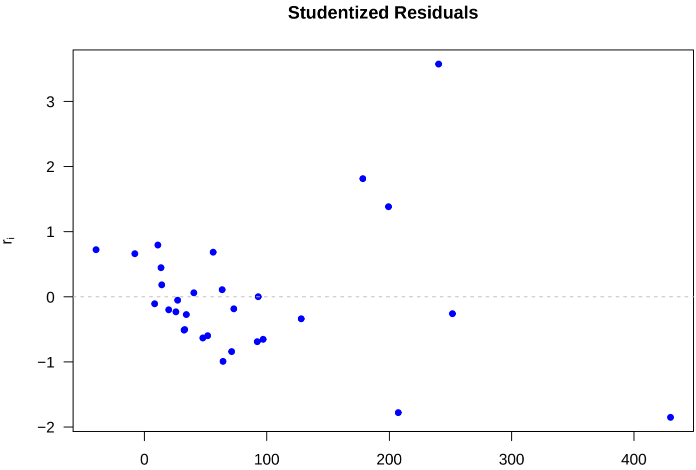


Standardized Residuals

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 **standardized 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

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



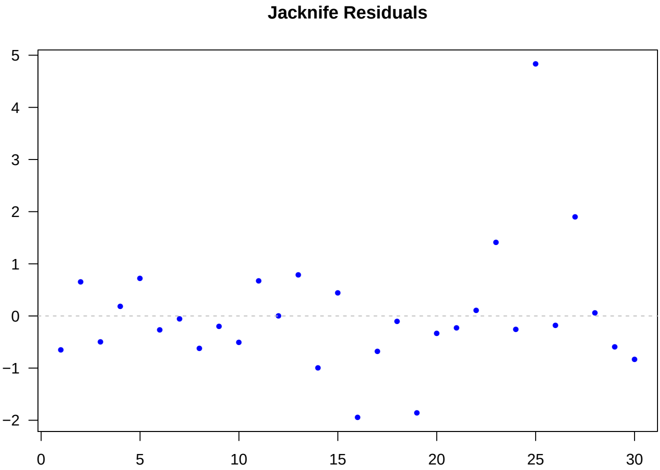
Studentized (Jackknife) Residuals

- 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
  Var$(\hat{y}_{i(i)} - y_i) = \sigma^2_{(i)} \left(1 + \boldsymbol{x}_i^T (\boldsymbol{X}_{(i)}^T \boldsymbol{X}_{(i)})^{-1} \boldsymbol{x}_i\right) = \sigma^2_{(i)}(1 - h_i)$
- Define the **Studentized (Jackknife) Residuals** as

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

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

Studentized (Jackknife) Residuals of `Species` $\sim$ `Elev` $+$ `Adj`



Identifying Influential Observations: Cook's Distance

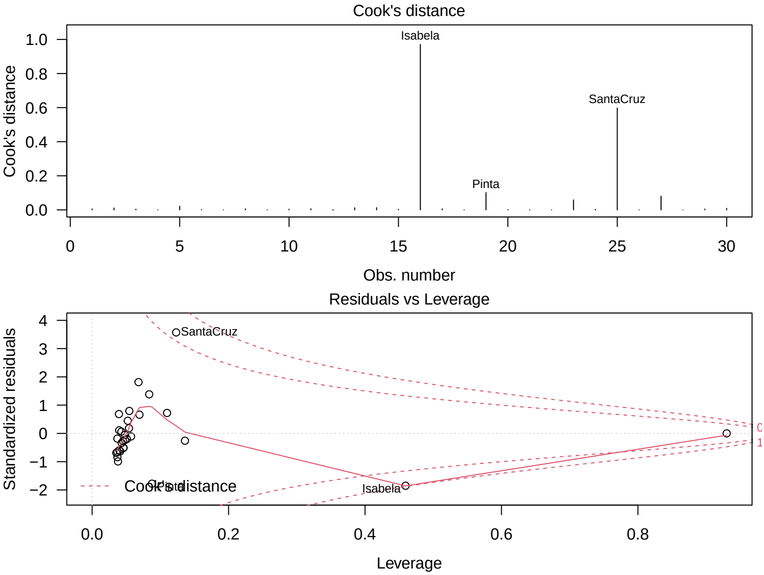
Cook's Distance quantifies how much the predicted values change when a particular observation is excluded from the analysis.

- Cook's distance measure (D_i) is defined as:

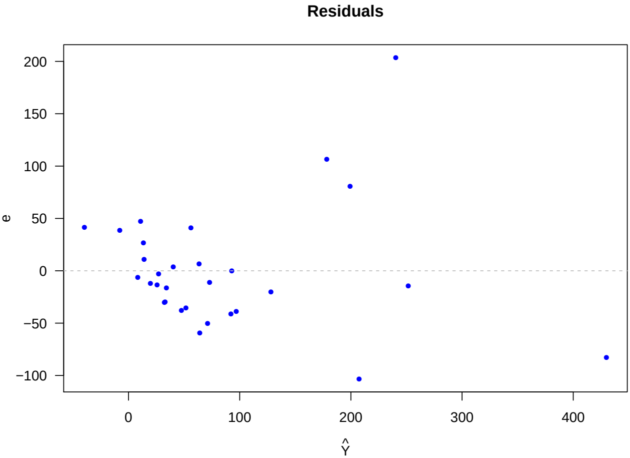
$$D_i = \frac{(y_i - \hat{y}_i)^2}{p \times \text{MSE}} \left(\frac{h_i}{(1 - h_i)^2} \right)$$

- Cook's Distance considers both leverage and residual, providing a broader measure of influence
- Here are the guidelines commonly used:
  1. If $D_i > 0.5$, then the i$^{\text{th}}$ data point is worthy of further investigation as it may be influential
  2. If $D_i > 1$, then the i$^{\text{th}}$ data point is quite likely to be influential

Cook's Distance of `Species` ~ `Elev` + `Adj`



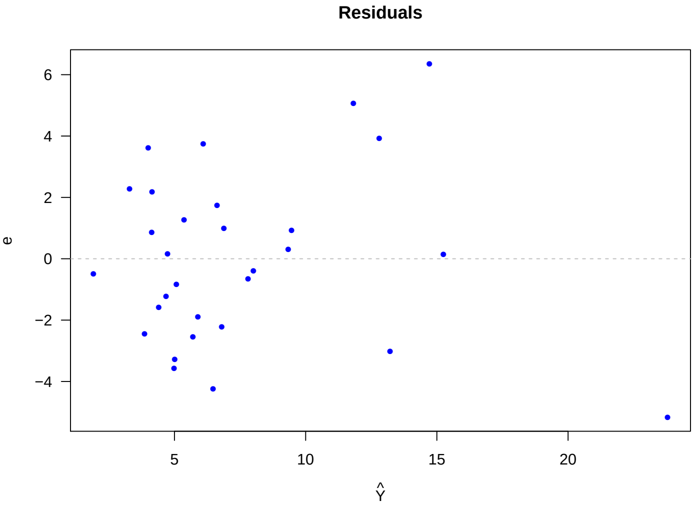
Residual Plot of `Species` ~ `Elev` + `Adj`



Such a residual plot suggests a violation of constant variance

Residual Plot After Square Root Transformation

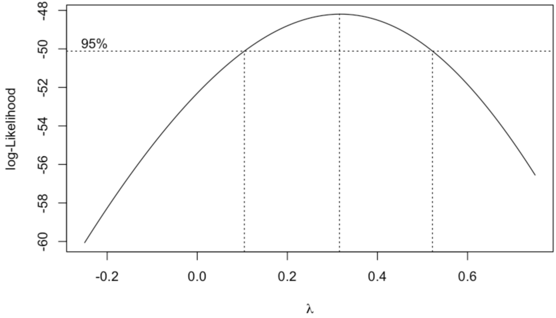
$$\sqrt{\text{Species}} \sim \text{Elev} + \text{Adj}$$



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

These slides cover:

- General Linear F-Test provides a unifying framework for hypothesis tests
- Making predictions and quantifying prediction uncertainty
- Multicollinearity and its implications for MLR
- 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

R Functions to Know

- `anova` for model comparison based on F-test
- `predict`: obtain predicted values from a fitted model
- `vif` under the `faraway` library: computes the variance inflation factors
- `regsubsets` in the `leaps` library and `step` for model selection
- `influence.measures` includes a suite of functions (`hatvalues`, `rstandard`, `rstudent`, `cooks.distance`) for computing regression diagnostics
- `boxcox` in the `MASS` library for performing a Box-Cox transformation