

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

Multiple Linear Regression II

Notes

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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**

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Multiple Linear

4.1

Notes

4 Reject H_0 if $F^* > F_{1-\alpha,p-1,n-p}$

[Both tests are special cases of](#page-14-0) General Linear ^F-test

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General Linear F**-Test**

- Comparison of a "full model" and "reduced model" that involves **a subset of full model predictors**
- \bullet Consider a full model with k predictors and reduced model with ℓ predictors $(\ell < k)$
- Test statistic: $F^* = \frac{(SSE_{\text{reduce}} SSE_{\text{full}})/(k-\ell)}{SSE_{\text{full}}/(n-k-1)}$ ⇒ Testing H_0 that the regression coefficients for the extra variables are all zero
	- Example 1: x_1, x_2, \dots, x_{p-1} vs. intercept only ⇒ Overall F-test
	- Example 2: x_j , $1 \le j \le p-1$ vs. intercept only \Rightarrow t-test for β_j
	- Example 3: x_1, x_2, x_3, x_4 vs. x_1, x_3 ⇒ $H_0: \beta_2 = \beta_4 = 0$

Multiple Linear Regression II General Linear F -Test

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Geometric Illustration of General Linear F**-Test**

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

General Linear F -Test

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Multiple Linear Regression II

Notes

Species Diversity on the Galapagos Islands: Full Model

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

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Species Diversity on the Galapagos Islands: Reduce Model

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Multiple Linear

Notes

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Performing a General Linear F**-Test**

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

> anova(gala_fit1, gala_fit2)
Analysis of Variance Table

Multiple Linear Regression II

Visualizing p**-value**

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Another Example of General Linear F**-Test**

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Multiple Linear Regression II

General Linear F -Test

Notes

Performing a General Linear F**-Test**

• Null and alternative hypotheses:

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

- $F^* = \frac{(100003 89231)/(5-2)}{89231/(30-5-1)} = 0.9657$
- **•** *p*-value: $\mathbb{P}[F > 0.9657] = 0.425$, where $F \sim F_{3,24}$

> anova(reduced, full)
Analysis of Variance Table

Model 1: Species \sim Elevation + Adjacent Model 2: Species ~ Area + Elevation + Nearest + Scruz + Adjacent
Res.Df RSS Df Sum of Sq F Pr(>F) $\mathbf 1$ 27 100003 24 89231 3 10772 0.9657 0.425 \overline{z}

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Multiple Linear Regression Prediction

Given a new set of predictors, $x_0 = (1, x_{0,1}, x_{0,2}, \cdots, x_{0,p-1})^{\mathrm{T}}$, the predicted response is

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

Again, we can use matrix representation to simplify the notation

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

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

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

Multiple Linear Regression II

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Two Kinds of Predictions

There are two kinds of predictions can be made for a given 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 $\hat{y}_0 = \boldsymbol{x}_0^{\text{T}} \hat{\boldsymbol{\beta}}$

Predicting the mean response: Since $E(y_0) = x_0^{\mathrm{T}}\beta$, there we have the predicted mean response

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

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 $\text{Var}(\hat{\boldsymbol{\beta}})$ = $\sigma^2\left(\boldsymbol{X}^{\text{T}}\boldsymbol{X}\right)^{-1}$. Therefore we have

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

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

• Predicting a future response y_0 :

$$
\boldsymbol{x}_0^{\mathrm{T}} \boldsymbol{\hat{\beta}} \pm t_{1-\alpha/2,n-p} \times \hat{\sigma} \sqrt{\frac{1}{\underbrace{1+x_0^{\mathrm{T}} \left(\boldsymbol{X}^{\mathrm{T}} \boldsymbol{X} \right)^{-1} \boldsymbol{x}_0}}}{\text{accounting for }\varepsilon}
$$

• Predicting the mean response $E(y_0)$:

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

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Prediction

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Notes

Example: Predicting Body Fat Cont'd

- \bullet Calculate the median for each predictor to get x_0
- **2** Compute the predicted value $\hat{y}_0 = \boldsymbol{x}_0^{\text{T}} \hat{\boldsymbol{\beta}}$
- ³ Quantify the prediction uncertainty

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Multicollinearity

Multicollinearity

Multiple Linear Regression II

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$> cor(sim1)$

 $\begin{array}{@{}c@{\hspace{1em}}c@{\hspace{$ 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 \Rightarrow the matrix $X^T X$ is nearly singular
- Statistical issues/consequences
	- θ 's are not well estimated \Rightarrow spurious regression coefficient estimates
	- R^2 and predicted values are usually okay even with multicollinearity

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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 $\varepsilon \sim N(0, 1)$ 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

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Scatter Plot: x_1 **vs.** x_2

Multicollinearity

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Multiple Linear Regression II

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Model 1 Fit

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

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 0.1 ' ' 1

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Model 2 Fit

 $Call:$ $lm(formula = Y ~ x1)$

Residuals: 10 Median Min 1Q Median 3Q Max
-2.09663 -0.67031 -0.07229 0.87881 1.49739

Coefficients:

Estimate Std. Error t value Pr(>|t|)

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 *** II.

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

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Multiple Linear Regression II

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Notes

Takeaways

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

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

$\underset{\text{in} \text{(formula = Y - X1)}}{\text{Model 2 fit:}}$

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

Coefficients :
Estimate Std. Error t value Pr(>ItI)
- 4.0347 - 0.1763 - 22.888 - 2e-16 ***
- 1.4293 - 0.1955 - 7.311 5.84e-08 *** (Intercept)
X1 ---
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

Multicollinearity Recall the true model: $Y = 4 + 0.8x_1 + 0.6x_2 + \varepsilon$, where $\varepsilon \sim N(0,1)$, x_1 and x_2 are positively correlated with $\rho = 0.9$ **Summary:** \bullet β 's are not well estimated

- in model 1 [⇒] 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)

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

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.

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Model Selection in Multiple Linear Regression

Multiple Linear Regression Model:

 $Y=\beta_0+\beta_1x_1+\beta_2x_2+\cdots+\beta_{p-1}x_{p-1}+\varepsilon, \quad \varepsilon\overset{i.i.d.}{\sim}\mathrm{N}\big(0,\sigma^2\big)$

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

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

−10 −5 0 5 10 40 100 120 x Obs Ubderfit Overfit 0 20

−10 −5 0 5 10

x

−10 −5 0 5 10

x

An Example of Bias and Variance Tradeoff

True

−60 −40 −20

> 0 1

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Notes

Balancing Bias And Variance: Mallows' C_p **Criterion** A good model should balance **bias** and **variance** to get good predictions

$$
(\hat{Y}_i - \mu_i)^2 = (\hat{Y}_i - \mathbb{E}(\hat{Y}_i) + \mathbb{E}(\hat{Y}_i) - \mu_i)^2
$$

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

where $\mu_i = \mathbb{E}(Y_i | X_i = x_i)$ Mean squared prediction error (MSPE): $\sum_{i=1}^{n} \sigma_{\hat{Y}_i}^2 + \sum_{i=1}^{n} (\mathbb{E}(\hat{Y}_i) - \mu_i)^2$

\bullet C_p criterion measure:

$$
\Gamma_p = \frac{\sum_{i=1}^{n} \sigma_{\hat{Y}_i}^2 + \sum_{i=1}^{n} (\mathbb{E}(\hat{Y}_i) - \mu_i)^2}{\sigma^2}
$$

$$
= \frac{\sum \text{Var}_{\text{pred}} + \sum \text{Bias}^2}{\text{Var}_{\text{error}}}
$$

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[Notes](#page-0-0)

C^p **Criterion**

 C_p statistic:

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

- When model is correct $E(C_p) \approx p$
- \bullet 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

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Multiple Linear Regression II

MATHEMATICAL AND

Model Selection

Notes

Adjusted R ² **Criterion**

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

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

- Choose model which maximizes $R_{\sf adj}^2$
- Same approach as choosing model with smallest MSE

Notes

Information criteria

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

Akaike's information criterion (AIC)

$$
n\log\left(\frac{\text{SSE}_k}{n}\right) + 2k
$$

• Bayesian information criterion (BIC)

$$
n\log\left(\frac{\text{SSE}_k}{n}\right) + k\log(n)
$$

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

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

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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

Contract

Notes

Model Assumptions

Model:

$Y=\beta_0+\beta_1x_1+\beta_2x_2+\cdots+\beta_{p-1}x_{p-1}+\varepsilon,\quad \varepsilon\overset{i.i.d.}{\sim}\mathrm{N}\big(0,\sigma^2\big)$

We make the following assumptions:

· Linearity:

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

Errors have constant variance, are independent, and normally distributed

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

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We will revisit this in the end of the lecture

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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

 \bullet 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
- $\frac{1}{n} \le h_i \le 1$, $1 \le i \le n$ 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

Regression II MATHEMATICAL AND
STATISTICAL SCIENCE Model Diagnostics

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Multiple Linear

Multiple Linear

Leverage Values of Species ∼ **Elev** + **Adj**

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Notes

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Standardized Residuals

As we have seen $\text{Var}(e_i) = \sigma^2(1-h_i)$, 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 $\text{Corr}(r_i, r_j)$ tends to be small

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Multiple Linear Regression II

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Studentized (Jackknife) Residuals

- \bullet For a given model, exclude the observation i and recompute $\hat{\beta}_{(i)}$, $\hat{\sigma}_{(i)}$ 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

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

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

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Studentized (Jackknife) Residuals of Species ∼ **Elev** + **Adj**

Multiple Linear Regression II

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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.

 \bullet 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:
	- \bullet If $D_i > 0.5$, then the ith data point is worthy of further investigation as it may be influential
	- **2** If $D_i > 1$, then the ith data point is quite likely to be influential

Multiple Linear Regression II

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Notes

Residual Plot of Species [∼] **Elev** ⁺ **Adj**

Multiple Linear

variance

Residual Plot After Square Root Transformation

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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

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:

- \bullet 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
- \bullet 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

Notes

Notes

^R Functions to Know

- \bullet 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

Transformation

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Multiple Linear Regression II

Non-Constant Variance & **Transformation**

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Multiple Linear Regression II

Non-Constant Variance & **Transformation**

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