

Lecture 3


Multiple Linear Regression I

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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Multiple Linear Regression
Estimation & Inference
Assessing Model Fit


3.1

Notes

Agenda

- 1 Multiple Linear Regression
- 2 Estimation & Inference
- 3 Assessing Model Fit

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Multiple Regression Analysis

Goal: To model the population relationship between two or more predictors (X's) and a response (Y').


$$\text{Model: } Y' = f(x) + \varepsilon.$$

Example: Species diversity on the Galapagos Islands.

We are interested in studying the relationship between the number of plant species (Species) and the following geographic variables: Area, Elevation, Nearest, Scruz, Adjacent.



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Data: Species Diversity on the Galapagos Islands

	Species	Endemics	Area	Elevation	Nearest	Scruz	Adjacent
Baltra	58	23	25.09	346	0.6	0.6	1.84
Bartolome	31	21	1.24	109	0.6	26.3	572.33
Caldwell	3	3	0.21	114	2.8	58.7	0.78
Champion	25	9	0.10	46	1.9	47.4	0.18
Coamano	2	1	0.05	77	1.9	1.9	903.82
Daphne.Major	18	11	0.34	119	8.0	8.0	1.84
Daphne.Minor	24	0	0.08	93	6.0	12.0	0.34
Darwin	10	7	2.33	168	34.1	290.2	2.85
Eden	8	4	0.03	71	0.4	0.4	17.95
Enderby	2	2	0.18	112	2.6	50.2	0.10
Espanola	97	26	58.27	198	1.1	88.3	0.57
Fernandina	93	35	634.49	1494	4.3	95.3	4669.32
Gardner1	58	17	0.57	49	1.1	93.1	58.27
Gardner2	5	4	0.78	227	4.6	62.2	0.21
Genovesa	40	19	17.35	76	47.4	92.2	129.49
Isabela	347	89	4669.32	1707	0.7	28.1	634.49
Marchena	51	23	129.49	343	29.1	85.9	59.56
Onslow	2	2	0.01	25	3.3	45.9	0.10
Pinta	104	37	59.56	777	29.1	119.6	129.49
Pinzon	108	33	17.95	458	10.7	10.7	0.03
Las.Plazas	12	9	0.23	94	0.5	0.6	25.09
Rabida	70	30	4.89	367	4.4	24.4	572.33
SanCristobal	280	65	551.62	716	45.2	66.6	0.57
SanSalvador	237	81	572.33	906	0.2	19.8	4.89
SantaCruz	444	95	903.82	864	0.6	0.0	0.52
SantaFe	62	28	24.08	259	16.5	16.5	0.52
SantaMaria	285	73	170.92	640	2.6	49.2	0.10
Seymour	44	16	1.84	147	0.6	9.6	25.09
Tortuga	16	8	1.24	186	6.8	50.9	17.95
Wolf	21	12	2.85	253	34.1	254.7	2.33

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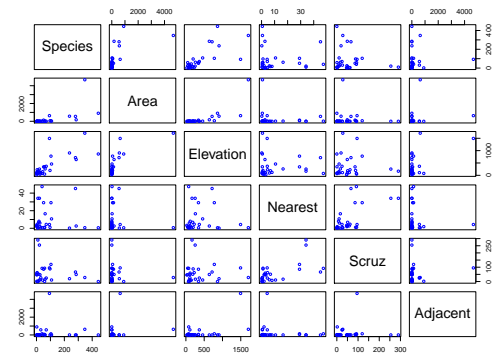
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How Do Geographic Variables Affect Species Diversity?



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Let's Take a Look at the Correlation Matrix

Here we compute the correlation coefficients between the response (Species) and predictors (all the geographic variables)

```
> round(cor(gala[, -2]), 3)
```

	Species	Area	Elevation	Nearest	Scruz	Adjacent
Species	1.000	0.618	0.738	-0.014	-0.171	0.026
Area	0.618	1.000	0.754	-0.111	-0.101	0.180
Elevation	0.738	0.754	1.000	-0.011	-0.015	0.536
Nearest	-0.014	-0.111	-0.011	1.000	0.615	-0.116
Scruz	-0.171	-0.101	-0.015	0.615	1.000	0.052
Adjacent	0.026	0.180	0.536	-0.116	0.052	1.000

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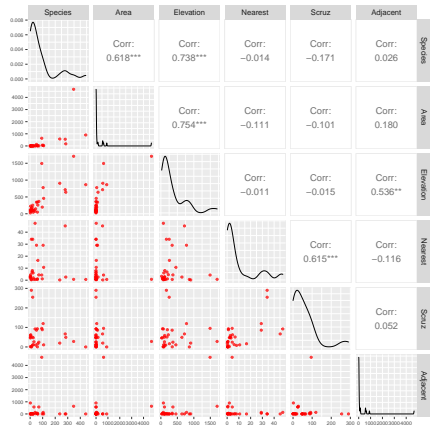
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Combining Two Pieces of Information in One Plot



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Multiple Linear Regression Model

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_{p-1} X_{p-1} + \varepsilon$$

- The above relationship holds for every individual in the population, and $E(\varepsilon) = 0$ and $Var(\varepsilon) = \sigma^2$
- The population of individual error terms (ε 's) follows normal distribution
- Observations are independent (true if individuals are selected randomly)
 $\Rightarrow \varepsilon \overset{i.i.d.}{\sim} N(0, \sigma^2)$

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Model 1: Species ~ Elevation

```
Call:
lm(formula = Species ~ Elevation, data = gala)

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
```

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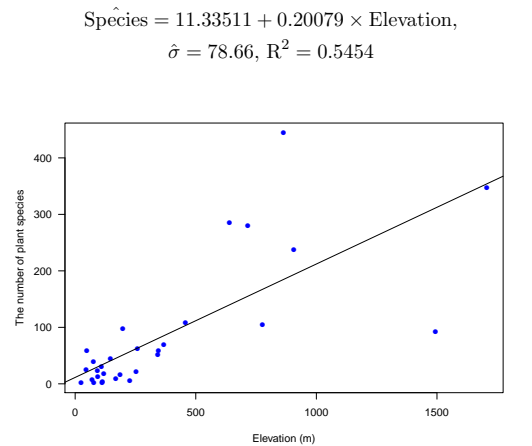
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Model 1 Fit



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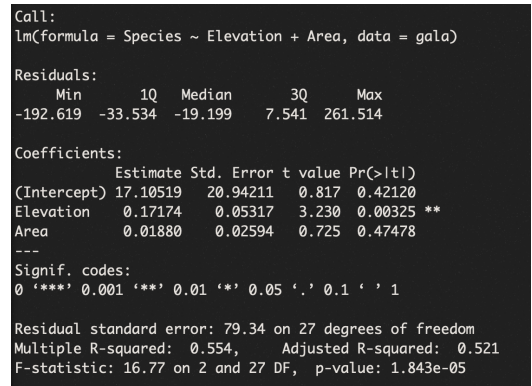
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Model 2: Species ~ Elevation + Area



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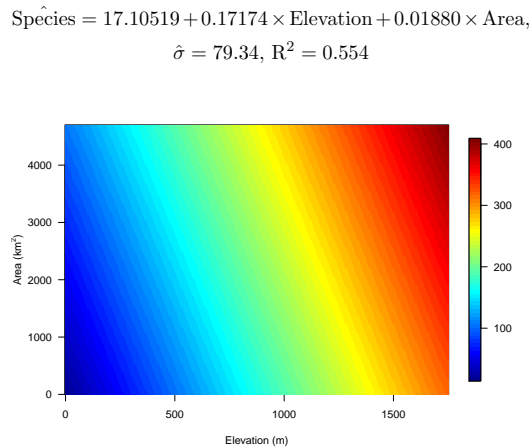
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Model 2 Fit



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Model 3: Species ~ Elevation + Area + Adjacent

```
Call:
lm(formula = Species ~ Elevation + Area + Adjacent, data = gala)

Residuals:
    Min       1Q   Median       3Q      Max
-124.064  -34.283   -8.733   27.972  195.973

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  -5.71893    16.90706   -0.338  0.73789
Elevation     0.31498     0.05211    6.044 2.2e-06 ***
Area         -0.02031     0.02181   -0.931  0.36034
Adjacent     -0.07528     0.01698   -4.434  0.00015 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 61.01 on 26 degrees of freedom
Multiple R-squared:  0.746,    Adjusted R-squared:  0.7167
F-statistic: 25.46 on 3 and 26 DF,  p-value: 6.683e-08
```

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“Full Model”

```
lm(formula = Species ~ Area + Elevation + Nearest + Scruz + Adjacent,
    data = gala)

Residuals:
    Min       1Q   Median       3Q      Max
-111.679  -34.898   -7.862   33.460   182.584

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  7.068221   19.154198    0.369  0.715351
Area        -0.023938    0.022422   -1.068  0.296318
Elevation     0.319465    0.053663    5.953 3.82e-06
Nearest      0.009144    1.054136    0.009  0.993151
Scruz        -0.240524    0.215402   -1.117  0.275208
Adjacent     -0.074805    0.017700   -4.226  0.000297

(Intercept)
Area
Elevation ***
Nearest
Scruz
Adjacent ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 60.98 on 24 degrees of freedom
Multiple R-squared:  0.7658,    Adjusted R-squared:  0.7171
F-statistic: 15.7 on 5 and 24 DF,  p-value: 6.838e-07
```

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MLR Topics

Similar to SLR, we will discuss

- Estimation
- Inference
- Diagnostics and Remedies

We will also discuss some new topics

- Model Selection
- Multicollinearity

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Multiple Linear Regression in Matrix Notation

Given the actual data, we can write MLR model as:

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} 1 & x_{1,1} & x_{2,1} & \cdots & x_{p-1,1} \\ 1 & x_{1,2} & x_{2,2} & \cdots & x_{p-1,2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{1,n} & x_{2,n} & \cdots & x_{p-1,n} \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_{p-1} \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{pmatrix}$$

It will be more convenient to put this in a matrix representation as:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

Error Sum of Squares (SSE)

$$= \sum_{i=1}^n \left(y_i - \left(\beta_0 + \sum_{j=1}^{p-1} \beta_j x_{j,i} \right) \right)^2 \text{ can be expressed as:}$$

$$(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

Next, we are going to find $\hat{\boldsymbol{\beta}} = (\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_{p-1})$ to minimize SSE as our estimate for $\boldsymbol{\beta} = (\beta_0, \beta_1, \dots, \beta_{p-1})$

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Estimating Regression Coefficients

We apply method of least squares to minimize $(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$ to obtain $\hat{\boldsymbol{\beta}}$

What is important is the **orthogonality**, which leads to the following:

- $\sum_i^n (y_i - \hat{y}_i) = 0$
- $\sum_i^n (y_i - \hat{y}_i) x_{1,i} = 0$
- \vdots
- $\sum_i^n (y_i - \hat{y}_i) x_{p-1,i} = 0$

Note: The first equation states that the mean of the residuals is 0, while the other equations indicate that the residuals are uncorrelated with the independent variables

The resulting least squares estimate is

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

(see LS_MLR.pdf for the derivation)

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Estimation of σ^2

- Fitted values:

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} = \mathbf{H}\mathbf{y}$$

- Residuals:

$$\mathbf{e} = \mathbf{y} - \hat{\mathbf{y}} = (\mathbf{I} - \mathbf{H})\mathbf{y}$$

- Similar as we did in SLR

$$\begin{aligned} \hat{\sigma}^2 &= \frac{\mathbf{e}^T \mathbf{e}}{n - p} \\ &= \frac{(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})^T (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})}{n - p} \\ &= \frac{\text{SSE}}{n - p} \\ &= \text{MSE} \end{aligned}$$

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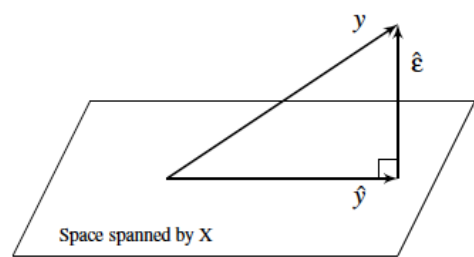
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Geometric Representation of Least Squares Estimation

Projecting the observed response y into a space spanned by X



Source: Linear Model with R 2nd Ed, Faraway, p. 15

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Notes

Regression with Numerical and Categorical Predictors

What if some of the predictors are categorical variables?


Example: Salaries for Professors Data Set

```
> head(Salaries)
  rank discipline yrs.since.phd yrs.service sex salary
1  Prof         B           19         18 Male 139750
2  Prof         B           20         16 Male 173200
3 AsstProf      B            4          3 Male  79750
4  Prof         B           45         39 Male 115000
5  Prof         B           40         41 Male 141500
6 AssocProf     B            6          6 Male  97000
```

We have three categorical variables, namely, rank, discipline, and sex.

⇒ We will need to create **dummy (indicator) variables** for those categorical variables

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Dummy Variable

For binary categorical variables:

$$x_{sex} = \begin{cases} 1 & \text{if sex = male,} \\ 0 & \text{if sex = female.} \end{cases}$$


$$x_{discip} = \begin{cases} 0 & \text{if discip = A,} \\ 1 & \text{if discip = B.} \end{cases}$$

For categorical variable with more than two categories:

$$x_{rank1} = \begin{cases} 0 & \text{if rank = Assistant Prof,} \\ 1 & \text{if rank = Associated Prof.} \end{cases}$$

$$x_{rank2} = \begin{cases} 0 & \text{if rank = Associated Prof,} \\ 1 & \text{if rank = Full Prof.} \end{cases}$$

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Design Matrix

```
> head(X)
      (Intercept) rankAssocProf rankProf disciplineB yrs.since.phd
1             1           0         1           1           19
2             1           0         1           1           20
3             1           0         0           1           4
4             1           0         1           1           45
5             1           0         1           1           40
6             1           1         0           1           6

      yrs.service sexMale
1             18         1
2             16         1
3              3         1
4             39         1
5             41         1
6              6         1
```

With the design matrix X , we can now use method of least squares to fit the model $Y = X\beta + \varepsilon$

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Model Fit: `lm(salary ~ rank + sex + discipline + yrs.since.phd)`

```
Coefficients:
      (Intercept)  67884.32   4536.89  14.963 < 2e-16 ***
disciplineB      13937.47   2346.53   5.940 6.32e-09 ***
rankAssocProf    13104.15   4167.31   3.145 0.00179 **
rankProf         46032.55   4240.12  10.856 < 2e-16 ***
sexMale          4349.37   3875.39   1.122 0.26242
yrs.since.phd     61.01    127.01    0.480 0.63124
---
Signif. codes:
  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 22660 on 391 degrees of freedom
Multiple R-squared: 0.4472, Adjusted R-squared: 0.4401
F-statistic: 63.27 on 5 and 391 DF, p-value: < 2.2e-16
```

Question: Interpretation of the slopes of these dummy variables (e.g. $\beta_{rankAssocProf}$)? Interpretation of the intercept?

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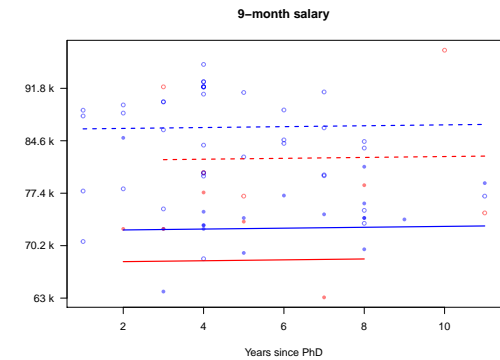
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Model Fit for Assistant Professors

Color	Line Type
Red: Female	—: Applied (discipline B)
Blue: Male	- - -: Theoretical (discipline A)



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Other Type of Predictor Variables: Polynomial regression

Suppose we would like to model the relationship between response Y and a predictor x as a p_{th} degree polynomial in x :

$$Y = \beta_0 + \beta_1x + \beta_2x^2 + \cdots + \beta_px^p + \varepsilon$$


Polynomial regression can be treated as a special case of multiple linear regression, with the design matrix taking the following form:

$$X = \begin{pmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^p \\ 1 & x_2 & x_2^2 & \cdots & x_2^p \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^p \end{pmatrix}$$

One can also include the interaction terms; for example:

$$Y = \beta_0 + \beta_1x_1 + \beta_2x_2 + \beta_3x_1^2 + \beta_4x_2^2 + \beta_5x_1x_2 + \varepsilon$$

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Transformed Response Variables

Consider the following models:


$$\log(Y) = \beta_0 + \beta_1x_1 + \beta_2x_2 + \varepsilon;$$
$$Y = \frac{1}{\beta_0 + \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \varepsilon},$$

both of which can be expressed as follws

$$Y^* = \beta_0 + \beta_1x_1 + \beta_2x_2 + \varepsilon;$$
$$Y^{**} = \beta_0 + \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \varepsilon,$$

respectively, where $Y^* = \log(Y)$, and $Y^{**} = 1/Y$.

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Analysis of Variance (ANOVA) Approach to Regression

Partitioning Sums of Squares


- Total sums of squares in response

$$SST = \sum_{i=1}^n (y_i - \bar{y})^2$$

- We can rewrite SST as

$$\sum_{i=1}^n (y_i - \bar{y})^2 = \sum_{i=1}^n (y_i - \hat{y}_i + \hat{y}_i - \bar{y})^2$$
$$= \underbrace{\sum_{i=1}^n (y_i - \hat{y}_i)^2}_{\text{"Error": SSE}} + \underbrace{\sum_{i=1}^n (\hat{y}_i - \bar{y})^2}_{\text{Model: SSR}}$$

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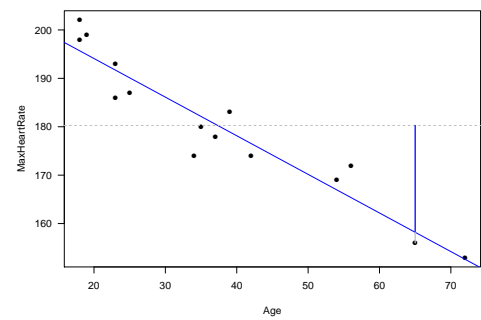
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Partitioning Total Sums of Squares: A Graphical Illustration



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ANOVA Table & F-Test

To answer the question: **Is at least one of the predictors** x_1, \dots, x_{p-1} **useful in predicting the response** y ?

Source	df	SS	MS	F-Value
Model	$p - 1$	SSR	$\text{MSR} = \text{SSR}/(p - 1)$	MSR/MSE
Error	$n - p$	SSE	$\text{MSE} = \text{SSE}/(n - p)$	
Total	$n - 1$	SST		

- **F-test:** Tests if the predictors $\{x_1, \dots, x_{p-1}\}$ collectively help explain the variation in y
 - $H_0 : \beta_1 = \beta_2 = \dots = \beta_{p-1} = 0$
 - $H_a : \text{at least one } \beta_k \neq 0, \quad 1 \leq k \leq p - 1$
 - $F^* = \frac{\text{MSR}}{\text{MSE}} = \frac{\text{SSR}/(p-1)}{\text{SSE}/(n-p)} \stackrel{H_0}{\sim} F_{p-1, n-p}$
 - Reject H_0 if $F^* > F_{1-\alpha, p-1, n-p}$

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Testing Individual Predictor

- We can show that $\hat{\beta} \sim N_p(\beta, \sigma^2 (X^T X)^{-1}) \Rightarrow \hat{\beta}_k \sim N(\beta_k, \sigma_{\hat{\beta}_k}^2)$
- Perform **t-test**:
 - $H_0 : \beta_k = 0$ vs. $H_a : \beta_k \neq 0$
 - $\frac{\hat{\beta}_k - \beta_k}{\text{se}(\hat{\beta}_k)} \sim t_{n-p} \Rightarrow t^* = \frac{\hat{\beta}_k}{\text{se}(\hat{\beta}_k)} \stackrel{H_0}{\sim} t_{n-p}$
 - Reject H_0 if $|t^*| > t_{1-\alpha/2, n-p}$
- Confidence interval for β_k :
$$\hat{\beta}_k \pm t_{1-\alpha/2, n-p} \text{se}(\hat{\beta}_k)$$

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Assessing Model Fit

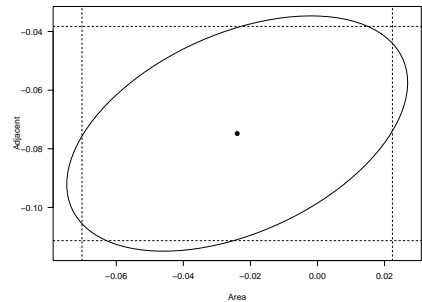
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Notes


Confidence Intervals and Confidence Ellipsoids

Comparing with individual confidence interval, confidence ellipsoids can provide additional information when inference with multiple parameters is of interest. A $100(1 - \alpha)\%$ confidence ellipsoid for β can be constructed using:

$$(\hat{\beta} - \beta)^T X^T X (\hat{\beta} - \beta) \leq p \hat{\sigma}^2 F_{p,n-p}^\alpha.$$



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Notes


Quantifying Model Fit using Coefficient of Determination R^2

- **Coefficient of determination** R^2 describes proportional of the variance in the response variable that is predictable from the predictors

$$R^2 = \frac{SSR}{SST} = 1 - \frac{SSE}{SST}, \quad 0 \leq R^2 \leq 1$$

- R^2 increases with the increasing p , the number of the predictors
 - Adjusted R^2 , denoted by $R^2_{adj} = 1 - \frac{SSE/(n-p)}{SST/(n-1)}$ attempts to account for p

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Notes

R^2 vs. R^2_{adj} Example

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

$$Y = 5 + 2x_1 + \varepsilon,$$

where $\varepsilon \sim N(0, 1)$ and x_1 and x_2 are independent to each other. Let's fit the following two models to the "data"


Model 1: $Y = \beta_0 + \beta_1 x_1 + \varepsilon^1$

Model 2: $Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon^2$

Question: Which model will "win" in terms of R^2 ?

Let's conduct a [Monte Carlo](#) simulation to study this

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Outline of Monte Carlo Simulation

- 1 Generating a large number (e.g., $M = 500$) of “data sets”, where each has exactly the same $\{x_{1,i}, x_{2,i}\}_{i=1}^n$ but different values of response $\{y_i = 5 + 2x_{1,i} + \varepsilon_i\}_{i=1}^n$
- 2 Fitting model 1: $Y = \beta_0 + \beta_1x_1 + \varepsilon^1$ (true model) and model 2: $Y = \beta_0 + \beta_1x_1 + \beta_2x_2 + \varepsilon^2$, respectively for each simulating data set and calculating their R^2 and R^2_{adj}
- 3 Summarizing $\{R^2_j\}_{j=1}^M$ and $\{R^2_{adj,j}\}_{j=1}^M$ for model 1 and model 2

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An Example of Model 1 Fit

```
> summary(fit1)

Call:
lm(formula = y ~ x1)

Residuals:
    Min       1Q   Median       3Q      Max
-1.6085 -0.5056 -0.2152  0.6932  2.0118

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  5.1720     0.1534   33.71  < 2e-16 ***
x1           1.8660     0.1589   11.74 2.47e-12 ***
---
Signif. codes:
  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.8393 on 28 degrees of freedom
Multiple R-squared:  0.8313,    Adjusted R-squared:  0.8253 
F-statistic: 138 on 1 and 28 DF,  p-value: 2.467e-12
```

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Notes

An Example of Model 2 Fit

```
> summary(fit2)

Call:
lm(formula = y ~ x1 + x2)

Residuals:
    Min       1Q   Median       3Q      Max
-1.3926 -0.5775 -0.1383  0.5229  1.8385

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  5.1792     0.1518   34.109 < 2e-16 ***
x1           1.8994     0.1593   11.923 2.88e-12 ***
x2          -0.2289     0.1797   -1.274  0.213
---
Signif. codes:
  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.8301 on 27 degrees of freedom
Multiple R-squared:  0.8408,    Adjusted R-squared:  0.8291 
F-statistic: 71.32 on 2 and 27 DF,  p-value: 1.677e-11
```

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Multiple Linear Regression

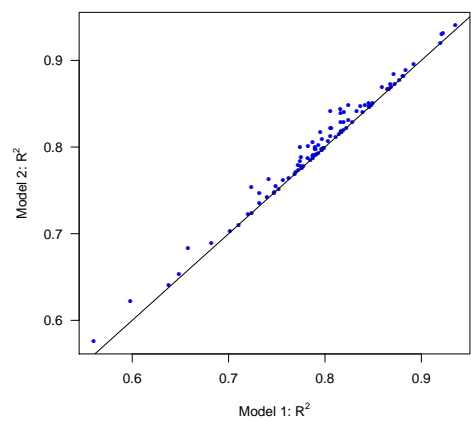
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Notes

R^2 : Model 1 vs. Model 2



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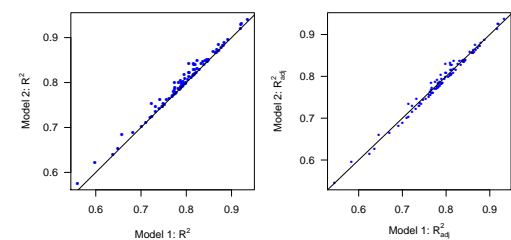
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Notes

R^2_{adj} : Model 1 vs. Model 2



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Notes

Takeaways:

- R^2 always pick the more “complex” model (i.e., with more predictors), even the simpler model is the true model
- R^2_{adj} has a better chance to pick the “right” model

Summary

These slides cover:

- Multiple Linear Regression: Model and Parameter Estimation
- Analysis of Covariance to handle situations where some predictors are categorical; Polynomial Regression, where polynomial terms are added to increase model flexibility
- Inference: F -test and t -test; Confidence intervals/ellipsoids
- Assessing Model Fit: R^2 and R^2_{adj}
- Monte Carlo Simulation

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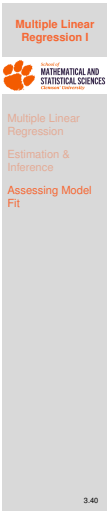
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Notes

R Functions to Know

- `image.plot` in the `fields` library and `scatter3D` in the `plot3D` library for visualization
- `anova` for computing the ANOVA table
- Use `*` to create interaction terms in `lm`
- Use `I(x)` or `poly(x, df)` to create polynomial terms



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