Lecture 3

Multiple Linear Regression: Inference and Prediction

Reading: Faraway 2014 Chapters 3.1-3.2; 3.5; 4.1-4.2; 4.4; 7.3. ISLR 2021 Chapter 3.2

DSA 8020 Statistical Methods II

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Agenda

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

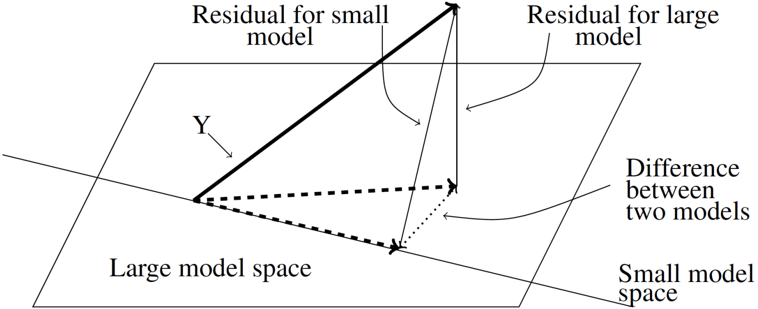
- t-Test: Testing one predictor
  1. **Null/Alternative Hypotheses**: $H_0 : \beta_j = 0$ vs. $H_a : \beta_j \neq 0$
  2. **Test Statistic**: $t^* = \frac{\hat{\beta}_j - 0}{SE(\hat{\beta}_j)}$
  3. Reject H_0 if $|t^*| > t_{1-\alpha/2, n-p}$
- Overall F-Test: Test of all the predictors
  1. $H_0 : \beta_1 = \beta_2 = \cdots = \beta_{p-1} = 0$
  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
  - Example 2: $x_j, 1 \leq j \leq p-1$ vs. intercept only $\Rightarrow$ t-test for β_j
  - Example 3: x_1, x_2, x_3, x_4 vs. x_1, x_3 $\Rightarrow$ $H_0 : \beta_2 = \beta_4 = 0$

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
```

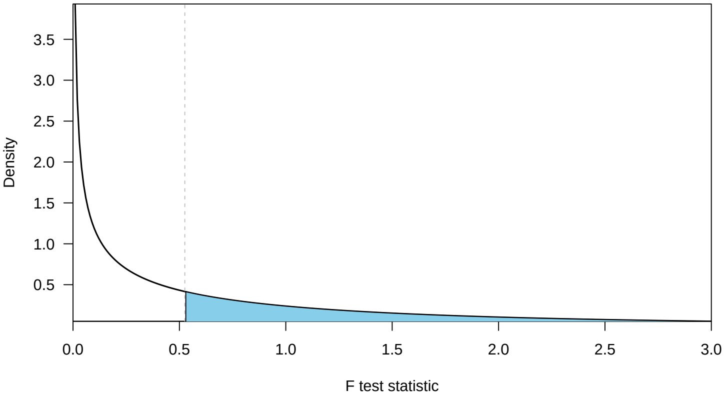
Performing a General Linear F-Test

- $H_0 : \beta_{\texttt{Area}} = 0$ vs. $H_a : \beta_{\texttt{Area}} \neq 0$
- $F^* = \frac{(173254-169947)/(2-1)}{169947/(30-2-1)} = 0.5254$
- P-value: $\mathrm{P}[F > 0.5254] = 0.4748$, 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 Model

```
> 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
```

Another Example of General Linear F-Test: Reduced Model


```
> 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:

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

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

- p-value: $\mathrm{P}[F > 0.9657] = 0.425$, 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 22 of slides 2, 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:**

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

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

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

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
```

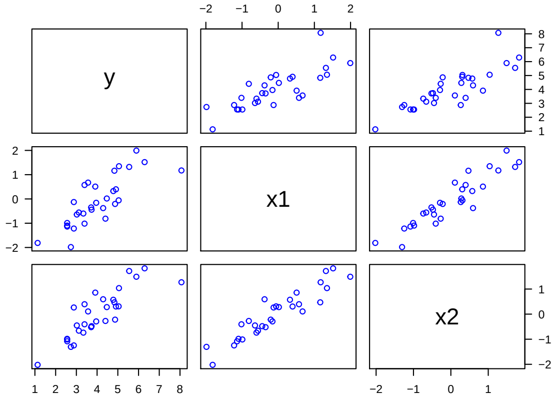
What is our prediction for the future response of a "typical" (e.g., each predictor takes its median value) man?

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

An Simulated Example

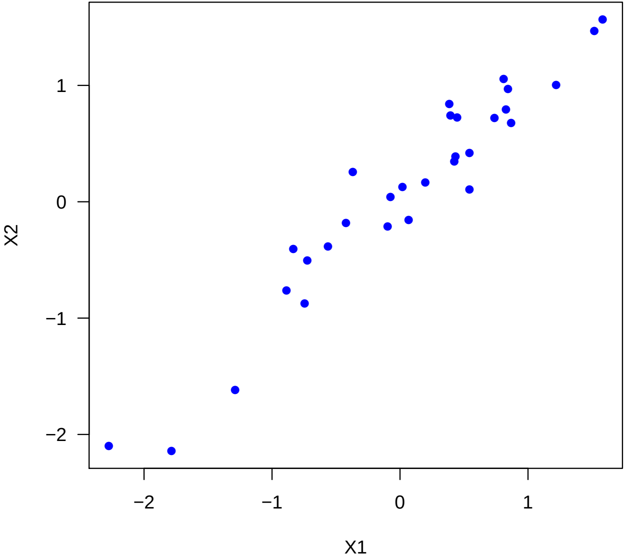
Suppose the true relationship between response y and predictors (x_1, x_2) is

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

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 
-1.91369 -0.73658  0.05475  0.87080  1.55150 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
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```

Model 2 fit:

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

Residuals:
     Min       1Q   Median       3Q      Max 
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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
```

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
- 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.

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

`R` commands:

- `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