

Model Accuracy

Statistics for Data Science II

Introduction

Recall the linear model,

$$y = \beta_0 + \beta_1 x_1 + \dots + \beta_k x_k + \varepsilon$$

Even if we know the true parameters (β_0 , β_1 , etc.), the linear model will not perfectly fit the data.

Thus, when constructing a model, we want to measure the model fit.

We can assess this with two quantities:

Residual standard error (RSE)

 R^2 statistic

Residuals

Recall the residual,

$$e_i = y_i - \hat{y}_i$$

This measures the distance between the observed value (y) and the predicted value (\hat{y}) for every observation.

We can also calculate the residual sum of squares (RSS),

$$RSS = \sum_{i=1}^{n} e_i^2$$

WEST FLORIDA Residual Standard Error

Then, we can calculate the residual standard error (RSE).

$$RSE = \sqrt{\frac{1}{n-2}RSS} = \sqrt{\frac{1}{n-2}\sum_{i=1}^{n}e_i^2}$$

The RSE estimates the standard deviation of ε .

We can actually pull this from the ANOVA table:

$$RSE = \sqrt{MSE}$$

Example:

Recall the models from the previous lecture,

```
\begin{aligned} &\text{M1:} \hat{y} = 13.04 + 0.14 \\ &\text{flipper} - 7.44 \\ &\text{Chinstrap} - 33.52 \\ &\text{Gentoo} + 0.09 \\ &\text{(flipper} \times \\ &\text{Chinstrap}) + 0.18 \\ &\text{(flipper} \times \\ &\text{Gentoo}) \\ &\text{M2:} \hat{y} = 37.26 + 3.13 \\ &\text{male} + 9.32 \\ &\text{Chinstrap} + 8.31 \\ &\text{Gentoo} + 1.39 \\ &\text{male} \times \\ &\text{Chinstrap} + 0.78 \\ &\text{male} \times \\ &\text{Gentoo} \end{aligned}
```

 $\mathsf{M3:} \hat{y} = -26.75 + 0.34 \mathsf{flipper} + 0.01 \mathsf{body} \; \mathsf{mass} - 0.00003 (\mathsf{flipper} \times \mathsf{body} \; \mathsf{mass})$

Let's find the RSE for each model.

We can use either summary() or anova()

```
##
## Call:
## lm(formula = bill length mm ~ flipper length mm + species Chinstrap +
       species_Gentoo + species_Chinstrap:flipper_length_mm + species Gentoo:flipper length mm.
##
      data = data)
##
## Residuals:
     Min
             10 Median
                                Max
## -6 698 -1 703 0 036 1 566 12 439
##
## Coefficients:
                                     Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                                      13.0358
                                                  6.1840 2.11 0.03579 *
## flipper length mm
                                       0.1357
                                                 0 0325 4 17 0 000039 ***
## species_Chinstrap
                                      -7 4424
                                                 10.5683 -0.70 0.48180
## species Gentoo
                                     -33.5237 9.9202 -3.38 0.00081 ***
## flipper length mm:species Chinstrap
                                      0.0852
                                                 0.0545
                                                         1.56 0.11909
## flipper_length_mm:species Gentoo
                                       0.1776
                                                 0.0483
                                                           3 68 0 00027 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 2.55 on 327 degrees of freedom
## Multiple R-squared: 0.785, Adjusted R-squared: 0.782
## F-statistic: 239 on 5 and 327 DF. p-value: <2e-16
```

```
anova(m1)
## Analysis of Variance Table
##
## Response: bill length mm
##
                                       Df Sum Sq Mean Sq F value Pr(>F)
## flipper length mm
                                           4235
                                                   4235
                                                        649.67
                                                                < 2e-16 ***
                                                         513.88 < 2e-16 ***
## species Chinstrap
                                           3350
                                                   3350
## species_Gentoo
                                            124
                                                    124 19.05 0.000017 ***
## flipper_length_mm:species_Chinstrap
                                                         0.01 0.92647
## flipper_length_mm:species_Gentoo
                                             88
                                                     88
                                                         13.54 0.00027 ***
## Residuals
                                      327
                                           2132
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
    Notice that RSE = \sqrt{7} = 2.65 \neq 2.55
```

Example: M1

Beware that sometimes R rounds things displayed – we may want to save things as a tibble (or data frame) to see the true values.

```
print.data.frame(round(anova(m1), 4))
##
                                             Sum Sq Mean Sq F value Pr(>F)
  flipper_length_mm
                                        1 4235 0137 4235 0137 649 6737 0 0000
## species Chinstrap
                                          3349.7977 3349.7977 513.8768 0.0000
## species Gentoo
                                           124.1841
                                                    124.1841 19.0505 0.0000
## flipper_length_mm:species_Chinstrap
                                             0.0556
                                                       0.0556
                                                                0.0085 0.9265
## flipper length mm:species Gentoo
                                            88.2438 88.2438 13.5371 0.0003
## Residuals
                                      327 2131 6078
                                                       6.5187
                                                                    NA
                                                                           NΑ
```

Thus, we see that the MSE is not actually 7. Instead, it is 6.5187.

Now, we match the output from summary(): $\sqrt{6.5187} = 2.55$.

```
##
## Call:
## lm(formula = bill length mm ~ sex male + species Chinstrap +
      species_Gentoo + species_Chinstrap:sex_male + species_Gentoo:sex_male,
      data = data)
##
## Residuals:
     Min
             10 Median
## -5.790 -1.374 -0.064 1.210 11.426
##
## Coefficients:
##
                             Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                               37 258
                                           0.271 \ 137.47 < 2e-16 ***
## sex male
                                3.133
                                           0.383
                                                   8.17
                                                         6.6e-15 ***
## species Chinstrap
                                9.316
                                           0.481
                                                   19.38 < 2e-16 ***
## species Gentoo
                                8.306
                                           0.407
                                                   20.39 < 2e-16 ***
## sex male:species Chinstrap
                                1.388
                                           0.680
                                                   2.04
                                                           0.042 *
## sex male:species Gentoo
                                0.777
                                           0.572
                                                   1.36
                                                           0.175
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 2.32 on 327 degrees of freedom
## Multiple R-squared: 0.823, Adjusted R-squared: 0.821
## F-statistic: 305 on 5 and 327 DF, p-value: <2e-16
```

WEST FLORIDA Residual Standard Error

```
##
## Call:
## lm(formula = bill length mm ~ flipper length mm + body mass g +
      flipper length mm:body mass g, data = data)
##
## Residuals:
     Min
             10 Median 30
## -9 106 -2 746 -0 786 2 158 18 955
##
## Coefficients:
##
                                Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                               -2.68e+01 2.11e+01
                                                     -1.26 0.2068
## flipper length mm
                                3.39e-01
                                         1.07e-01
                                                      3.17
                                                            0.0016 **
## body_mass_g
                                5.86e-03
                                         4.84e-03
                                                    1.21
                                                            0.2270
## flipper length mm:body mass g -2.59e-05 2.34e-05
                                                     -1.10 0.2701
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 4.15 on 329 degrees of freedom
## Multiple R-squared: 0.43. Adjusted R-squared: 0.425
## F-statistic: 82.8 on 3 and 329 DF. p-value: <2e-16
```

Example:

Comparing the three models,

Model	Predictors	RSE
1	species, flipper length	2.55
2	species, sex	2.32
3	flipper length, body mass	4.15

In theory, the model with the smallest RSE is the "best fitting" ... but how different is 2.32 and 2.55?

university of R2 Statistic

The downside to using the RSE is that it takes on the units of Y.

This means we cannot define a "good" RSE.

We now turn to a proportion, the R^2 statistic.

 R^2 is the proportion of variance explained by the model.

Because it is a proportion, $R^2 \in [0,1]$ and is independent of the units of Y.

If $R^2 \to 0$, the model does not fit the data well; if $R^2 \to 1$, the model fits the data well.

Note that if $R^2 = 1$, all observations fall on the response surface.

UNIVERSITY of R² Statistic

To calculate R^2 , we need RSS as well as the total sum of squares (TSS),

$$\mathsf{RSS} = \sum_{i=1}^n e_i^2$$
 and $\mathsf{TSS} = \sum_{i=1}^n (y_i - \bar{y})^2$

Then.

$$R^2 = \frac{\mathsf{TSS} - \mathsf{RSS}}{\mathsf{TSS}} = 1 - \frac{\mathsf{RSS}}{\mathsf{TSS}}$$

Note that other places may have different language (using the ANOVA table),

$$R^2 = \frac{\mathsf{SSTot} - \mathsf{SSE}}{\mathsf{SSTot}} = 1 - \frac{\mathsf{SSReg}}{\mathsf{SSTot}}$$

Remember that we are partitioning the variability in Y (TSS, or SSTot) into two pieces:

The variability explained by the regression model (TSS - RSS, or SSReg) and the variability explained by outside sources (RSS, or SSE).

As predictors are added to the model, we necessarily increase SSReg / decrease SSE.

We want a measure of model fit that is resistant to this fluxuation.

$$R_{\text{adj}}^2 = 1 - \left(\frac{n-1}{n-k-1}\right) \left(1 - R^2\right)$$

Example:

Recall the models from the previous lecture,

$$M1: \hat{y} = 13.04 + 0.14 \text{flipper} - 7.44 \text{Chinstrap} - 33.52 \text{Gentoo} + 0.09 (\text{flipper} \times \text{Chinstrap}) + 0.18 (\text{flipper} \times \text{Gentoo})$$

$$\mathsf{M2:} \hat{y} = 37.26 + 3.13 \mathsf{male} + 9.32 \mathsf{Chinstrap} + 8.31 \mathsf{Gentoo} + 1.39 \mathsf{male} \times \mathsf{Chinstrap} + 0.78 \mathsf{male} \times \mathsf{Gentoo}$$

$$M3: \hat{y} = -26.75 + 0.34 \text{flipper} + 0.01 \text{body mass} - 0.00003 \text{(flipper} \times \text{body mass)}$$

Let's find the R_{adj}^2 for each model.

Again, we can use either summary() or anova()

```
##
## Call:
## lm(formula = bill length mm ~ flipper length mm + species Chinstrap +
      species Gentoo + species Chinstrap:flipper length mm + species Gentoo:flipper length mm,
##
##
      data = data)
##
## Residuals:
     Min
             10 Median
                                Max
## -6 698 -1 703 0 036 1 566 12 439
##
## Coefficients:
##
                                     Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                                      13.0358
                                                 6.1840 2.11 0.03579 *
## flipper length mm
                                      0.1357
                                                 0.0325 4.17 0.000039 ***
## species_Chinstrap
                                      -7 4424
                                                10.5683 -0.70 0.48180
## species Gentoo
                                     -33.5237 9.9202 -3.38 0.00081 ***
## flipper_length_mm:species_Chinstrap
                                     0.0852
                                                 0.0545
                                                        1.56 0.11909
## flipper length mm:species Gentoo
                                      0.1776
                                                 0.0483
                                                          3 68 0 00027 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.55 on 327 degrees of freedom
## Multiple R-squared: 0.785, Adjusted R-squared: 0.782
## F-statistic: 239 on 5 and 327 DF. p-value: <2e-16
```

```
##
## Call:
## lm(formula = bill length mm ~ sex male + species Chinstrap +
       species Gentoo + species Chinstrap: sex male + species Gentoo: sex male,
##
      data = data)
##
## Residuals:
     Min
             10 Median
                                 Max
## -5 790 -1 374 -0 064 1 210 11 426
##
## Coefficients:
                             Estimate Std. Error t value Pr(>|t|)
##
## (Intercept)
                               37.258
                                          0.271 \quad 137.47 \quad < 2e-16 ***
## sex male
                                3 133
                                      0.383 8.17 6.6e-15 ***
## species_Chinstrap
                                9.316
                                          0.481
                                                  19.38 < 2e-16 ***
## species Gentoo
                                8.306
                                          0.407
                                                  20.39 < 2e-16 ***
## sex male:species Chinstrap
                                1.388
                                           0.680
                                                   2.04
                                                         0.042 *
## sex male:species Gentoo
                                0.777
                                           0.572
                                                   1.36
                                                         0.175
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```
##
## Call:
## lm(formula = bill length mm ~ flipper length mm + body mass g +
      flipper length mm:body mass g, data = data)
##
## Residuals:
     Min
            10 Median 30 Max
## -9 106 -2 746 -0 786 2 158 18 955
##
## Coefficients:
##
                               Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                              -2.68e+01 2.11e+01 -1.26 0.2068
## flipper length mm
                               3.39e-01 1.07e-01 3.17 0.0016 **
## body_mass_g
                               5.86e-03 4.84e-03 1.21
                                                           0.2270
## flipper length mm:body mass g -2.59e-05 2.34e-05
                                                    -1.10 0.2701
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 4.15 on 329 degrees of freedom
## Multiple R-squared: 0.43, Adjusted R-squared: 0.425
## F-statistic: 82.8 on 3 and 329 DF. p-value: <2e-16
```



UNIVERSITY of R2 Statistic

Example:

Comparing the three models.

Model	Predictors	RSE	R_{adj}^2
1	species, flipper length	2.55	0.782
2	species, sex	2.32	0.821
3	flipper length, body mass	4.15	0.425

Model 2 accounts for the highest amount of variability in bill length at 82.1

Model 3 accounts for the lowest amount of variability in bill length at 42.5

UNIVERSITY of Further Considerations

Both RSE and $R_{\rm adi}^2$ are tools for us to assess how a model fits the data.

Sometimes, we just aren't going to have a high $R_{\rm adi}^2$ and we should be cautious about $R_{\rm adi}^2$ that are too high.

We should consider the change in $R_{\rm adi}^2$ when removing/adding predictors to the model.

How much "better" is the model with/without the term?

If it is going to complicate the analysis (e.g., an interaction term), is it worth the increase in $R_{\rm adi}^2$?