Cross-Validation and Bias-Variance

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Math 243: Stat Learning

October 14th, 2020

Outline

In today's class, we will. . .

- Discuss variability in error estimates
- Investigate methods of cross-validation (LOOCV and k-fold cv)
- Implement CV in R
- Investigate the Bias-Variance trade-off

Section 1

Cross Validation

Penguins!

The `penguins` data set from the `palmerpenguins` package collected by Dr. Kristen Gorman on several attributes of antarctic penguins:

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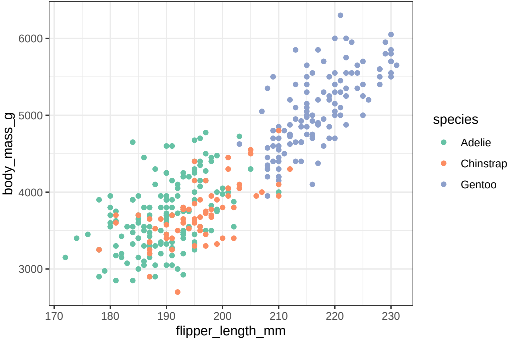
```
library(palmerpenguins)
data(penguins)
head(penguins)
```

```
## # A tibble: 6 x 8
##   species island bill_length_mm bill_depth_mm flipper_length_~ body_mass_g sex
##   <fct>   <fct>           <dbl>         <dbl>            <int>       <int> <fct>
## 1 Adelie  Torge~           39.1          18.7              181        3750 male
## 2 Adelie  Torge~           39.5          17.4              186        3800 fema~
## 3 Adelie  Torge~           40.3          18                195        3250 fema~
## 4 Adelie  Torge~           NA            NA                 NA          NA <NA>
## 5 Adelie  Torge~           36.7          19.3              193        3450 fema~
## 6 Adelie  Torge~           39.3          20.6              190        3650 male
## # ... with 1 more variable: year <int>
```

Penguin Species vs Body Mass and Flipper Length

Build LDA and QDA models for `species` as a function of `body_mass_g` and `flipper_length_mm`.

- Set a seed for reproducibility
- Use 70% of your data for training, and reserve remaining data for test.
- Record the error rates for each model on the google sheet on the course webpage



Example

```r
set.seed(1012)
penguins_train<-penguins %>% sample_frac(.7)
penguins_test<-penguins %>%  anti_join(penguins_train)

lda_mod<-lda(species ~ flipper_length_mm + body_mass_g, data = penguins_train)
qda_mod<-qda(species ~ flipper_length_mm + body_mass_g, data = penguins_train)

lda_pred<-predict(lda_mod, penguins_test)
qda_pred<-predict(qda_mod, penguins_test)
```

```r
lda_conf<-table(lda_pred$class, penguins_test$species)
lda_error<-(sum(lda_conf) - sum(diag(lda_conf)))/sum(lda_conf)

qda_conf<-table(qda_pred$class, penguins_test$species)
qda_error<-(sum(qda_conf) - sum(diag(qda_conf)))/sum(qda_conf)

data.frame(lda_error, qda_error)
```

```
##   lda_error qda_error
## 1 0.2673267 0.2376238
```

Leave One Out Cross Validation (LOOCV)

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- A single observation is randomly chosen as the test set
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For the *very* special case of least squares regression, the following formula for CV holds:

$$CV_{(n)} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i - \hat{y}_i}{1 - h_i}\right)^2 \qquad \text{where } h_i = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum_{j=1}^{n}(x_j - \bar{x})^2}$$

LOOCV in R

The `cv.glm()` function in the `boot` package can be used to perform LOOCV, and functions nearly identically to `glm()`.

```
library(boot)

penguins_nona <-penguins %>% drop_na()

my_glm<-glm(body_mass_g ~ flipper_length_mm , data = penguins_nona )
cv_error<- cv.glm(penguins_nona, my_glm)
cv_error$delta
```

```
## [1] 155563.6 155560.9
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- The cv.glm function produces a list with several components. For now, we are interesetd in the estimate for test MSE, which is the first entry of the delta attribute.
- Our CV RSE is the square root of the CV MSE:

$$\text{CV RSE}_{(n)} = \sqrt{MSE} = \sqrt{155563.6} = 394.4$$

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- Partition data into k sets of size n/k.
- Choose one subset of size n/k to be the test set, and remaining $k-1$ subsets to be training sets.
- Repeat for each subset of size n/k.

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- Note that LOOCV is a special case of k-fold CV when $k = n$.

k-fold CV in R

We again use the cv.glm() function in the boot package.

```
library(boot)
set.seed(1)

penguins_nona <-penguins %>% drop_na()

my_glm<-glm(body_mass_g ~ flipper_length_mm , data = penguins_nona  )
cv_error<- cv.glm(penguins_nona, my_glm, K = 10)
cv_error$delta
```

```
## [1] 155065.5 154997.3
```

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cv_error$delta
```

```
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```

- This gives a 10-fold CV RSE of

$$\mathrm{CV\,RSE}_{(10)} = \sqrt{CV}_{(10)} = \sqrt{155065.5} = 393.8$$

Cross Validation for LDA and QDA

Both `lda` and `qda` have a LOOCV argument in their respective functions:

```
my_lda<-lda(species ~ flipper_length_mm , data = penguins_nona  , CV = T)
```

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When `CV = T`, both `lda` and `qda` return a list of `class` (the prediction) and `posterior` (the probabilitiy), derived from the LOOCV analysis.

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```
head(my_lda$class)
```

```
## [1] Adelie Adelie Adelie Adelie Adelie Adelie
## Levels: Adelie Chinstrap Gentoo
```

```
head(my_lda$posterior)
```

```
##      Adelie  Chinstrap       Gentoo
## 1 0.9082461 0.09175317 7.235707e-07
## 2 0.8394852 0.16050009 1.475275e-05
## 3 0.6206141 0.37678880 2.597112e-03
## 4 0.6803584 0.31879476 8.468137e-04
## 5 0.7582377 0.24160938 1.528760e-04
## 6 0.9082461 0.09175317 7.235707e-07
```

Section 2

The Bias-Variance Trade-off

Example

See .html and .Rmd file on course webpage for live-coded notes