Cross Validation

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How to test models on the data?

- Sometimes we can build a model, then get more data to test the model.
- Most times we can't. We have the data we have.
- What to do?

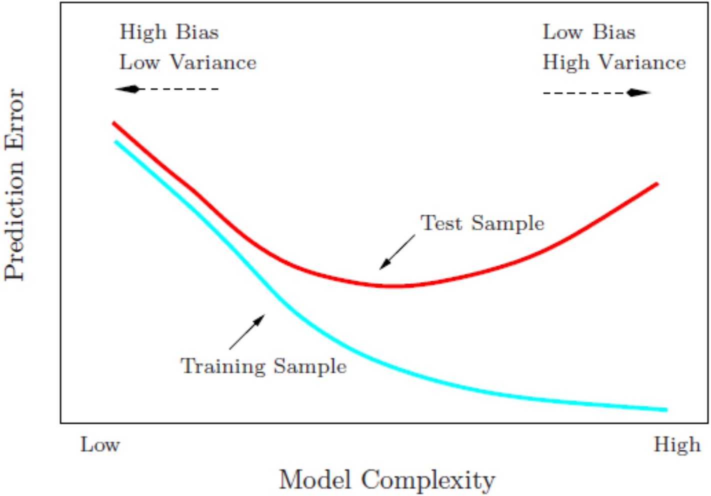
Hold-out

- Take some of the data and sequester it for testing
- Building the model ignores this data.
    - Can introduce bias if the test data is poorly selected.
- How to use the full data for training and testing?

Cross validation

- Divide the data into two non-overlapping parts:
  - Training set to build the model
  - Test set to test or validate the model
  - The model will naturally fit the training set better than the test set.
  - Use the performance test set to choose the best model
- Training error is $RSS/n = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \hat{y}_i\right)^2$ for y_i in training set
- Test error is error in test set $\frac{1}{m}\sum_{i=1}^{m}\left(y_i - \hat{y}_i\right)^2$

Training vs Test Error performance



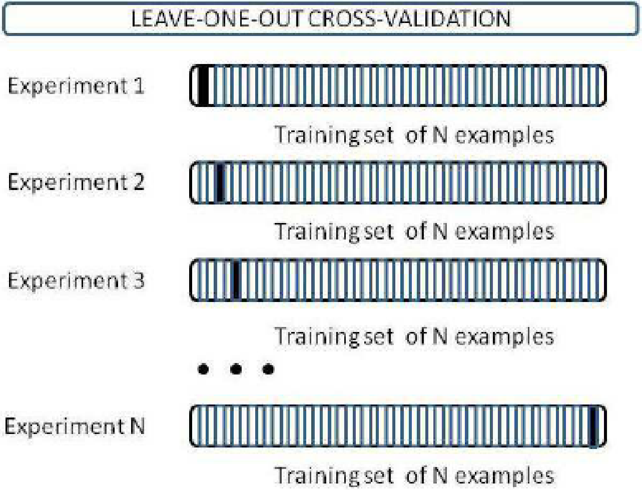
Cross validation

- In cross validation you successively divide the data into training and test sets
- Average test error over all iterations
- Choose model with lowest average test error
- Refit model using full data
- Average mean square error estimates the error on new data.

Leave one out cross validation

- Leave one out cross validation:
  - For each of the n observations, take the test set to be a single observation and the training set to be the other $n - 1$ observations.
  - Average performance across the test sets.
  - n total test iterations
- Small bias, large variance in estimating error on new data.

Leave one out cross validation



k-fold cross validation

- In k-fold cross validation you divide the data into k parts.
- Use each k parts as test sets, successively, and the remainder as training.
- Average performance across k test sets.
- As k increases the bias decreases and variance increases (in estimating error on new data).
    - Usually $k = 5$ or 10 is used.

k-fold cross validation

Cross validation in practice

- Let's apply cross validation to evaluate the performance of the forward and backward stepwise regression models we built last class.
- Forwards model: log(mpg) $\sim$ weight $+$ year $+$ origin $+$ horsepower
- Backwards model: log(mpg) $\sim$ cylinders $+$ displacement $+$ horsepower $+$ weight $+$ year $+$ origin

Cross validation in practice

```
n_folds = 10
fold = sample(1:n_folds, dim(Auto)[1],
              replace = TRUE)
forward_error = 0
backward_error = 0
```

Cross validation in practice

```
for(i in 1:n_folds){
  forward.lm = lm(log(mpg) ~ weight + year
                   + origin + horsepower,
                   data = Auto[-which(fold == i), ])
  forward_error = forward_error +
    mean((log(Auto$mpg[which(fold == i)]) -
            predict(forward.lm,
                     newdata = Auto[which(fold == i), ],
                     interval = "none"))^2)
}
```

Cross validation in practice

```
for(i in 1:n_folds){
  backward.lm = lm(log(mpg) ~ cylinders + displacement
                    + horsepower + weight + year + origin,
                   data = Auto[-which(fold == i), ])
  backward_error = backward_error +
    mean((log(Auto$mpg[which(fold == i)]) -
            predict(backward.lm,
                    newdata = Auto[which(fold == i), ],
                    interval = "none"))^2)
}
```

Cross validation in practice

```
forward_error
```

```
## [1] 0.1439297
```

```
backward_error
```

```
## [1] 0.1432977
```

Backwards error is lower, use larger model: log(mpg) $\sim$ cylinders + displacement + horsepower + weight + year + origin

Comparison with AIC, BIC, and adjusted R^2

```
backward.lm = lm(log(mpg) ~ cylinders + displacement
                   + horsepower + weight + year + origin,
                  data = Auto)
forward.lm = lm(log(mpg) ~ weight + year + origin
                  + horsepower, data = Auto)
```

Comparison with AIC, BIC, and adjusted R^2

```r
library(MASS)
AIC(forward.lm)
```

```
## [1] -544.6394
```

```r
AIC(backward.lm)
```

```
## [1] -547.6487
```

Comparison with AIC, BIC, and adjusted R^2

```
BIC(forward.lm)
```

```
## [1] -520.8118
```

```
BIC(backward.lm)
```

```
## [1] -515.8786
```

Comparison with AIC, BIC, and adjusted R^2

```r
summary(forward.lm)$adj.r.squared
```

```
## [1] 0.8760216
```

```r
summary(backward.lm)$adj.r.squared
```

```
## [1] 0.8775862
```