Model validation and selection

STEPHANIE J. SPIELMAN, PHD

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PLEASE INSTALL "pROC"

Recall our models

Linear models

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_n x_n + \varepsilon$$

Logistic regression

$$\Pr(success) = \frac{e^t}{1 + e^t}$$

$$t = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_n x_n + \varepsilon$$

Model validation and selection

Model Validation

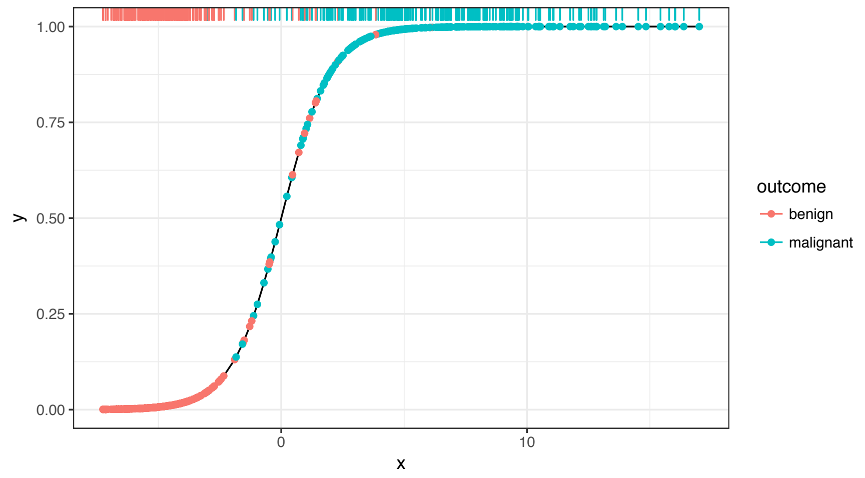
- What approaches can we use to evaluate the performance of a model?
- What metrics can we use to measure model performance?

Model Selection

- Given a set of possible models, how do we choose the "best" one?
- How do we choose predictors, in particular main vs. interaction effects?
- What metrics can we use to compare model performance?

Evaluating logistic regressions

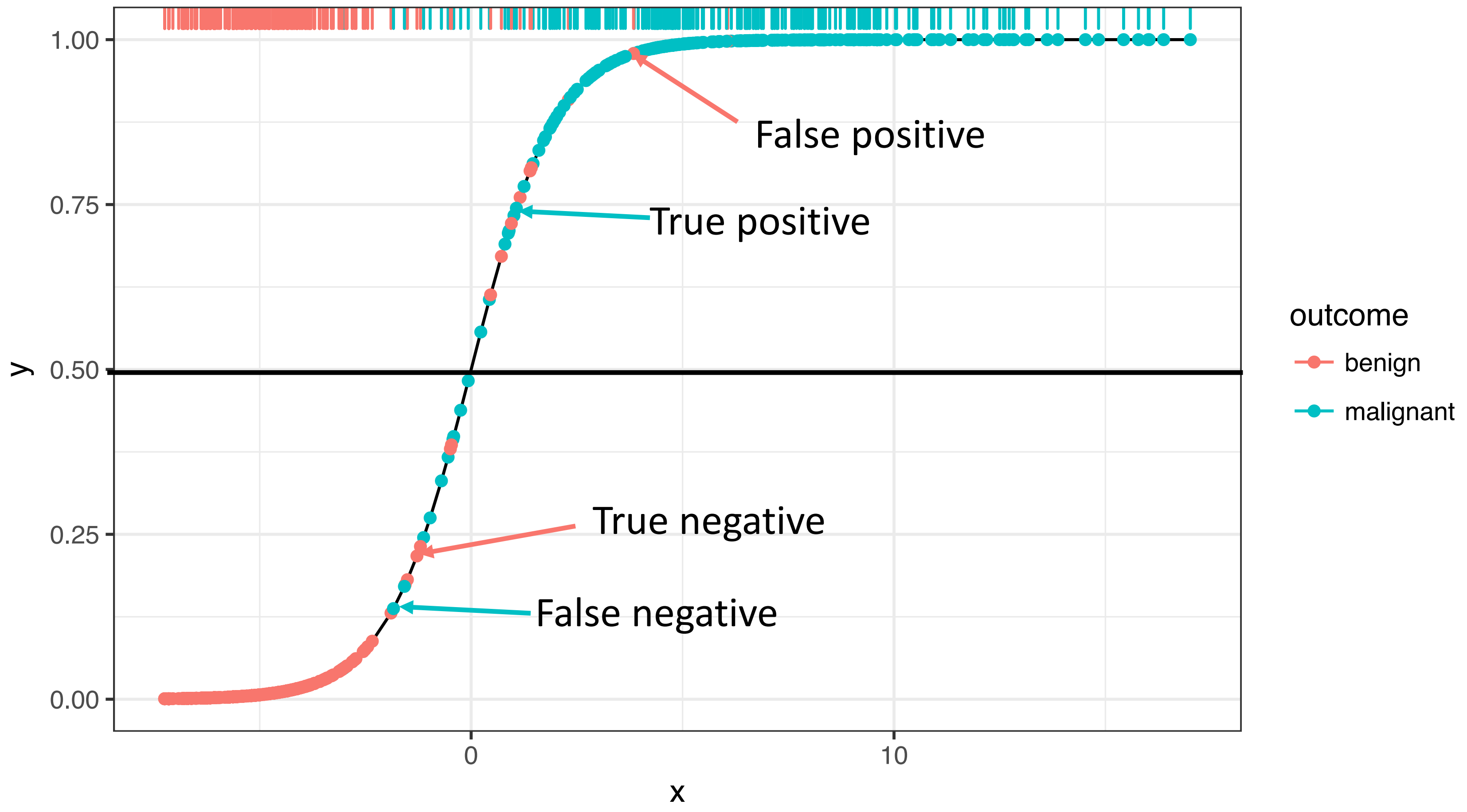
```
> model <- glm(outcome ~ ., data=biopsy, family=binomial)

> new.patient <- tibble(clump_thickness = 4,
                        uniform_cell_size = 2,
                        uniform_cell_shape = 7,
                        marg_adhesion = 3,
                        epithelial_cell_size = 8,
                        bare_nuclei = 1,
                        bland_chromatin =5,
                        normal_nucleoli = 2,
                        mitoses = 0)
> predict(model, new.patient, type = "response")
        1
0.2875157
```



Confusion matrix

		TRUTH	
		Negative (False)	**Positive (True)**
PREDICTION	**Positive (True)**	Type I error (False positive)	True positive
	Negative (False)	True negative	Type II Error (False negative)

Confusion matrix on the biopsy model



Emerging quantities

PREDICTION		TRUTH Negative (False)	TRUTH Positive (True)
	Positive (True)	FP	TP
	Negative (False)	TN	FN

True Positive Rate aka **Sensitivity** or **Recall**

TPR = TP/P = TP/(TP+FN)

True Negative Rate aka **Specificity**

TNR = TN/N = TN/(FP+TN)

False Positive Rate

FPR = FP/N = FP/(FP+TN) = 1 – TNR

Precision aka **Positive Predictive Value (PPV)**

TP/(TP+FP)

False discovery rate

FP/(FP+TP) = 1– PPV

Accuracy

(TP + TN) / (TP + TN + FP + FN)

Not enough for you?
https://en.wikipedia.org/wiki/Confusion_matrix

Calculate these qualities for biopsy model

```
> model <- glm(outcome ~ ., data=biopsy, family=binomial)


### Predict on all the rows
> predict(model, biopsy, type = "response") %>% as.data.frame()
               .
1   0.0160465814
2   0.9088086224
3   0.0081376226
4   0.7609349192
5   0.0181668485
6   0.9999736224
...
```

Calculate these qualities for biopsy model

```
> biopsy2 <- biopsy %>%
       mutate(pred = predict(model, biopsy, type = "response") )


### Let's say >=0.5 is a prediction of malignancy ###

> biopsy2 %>%
       mutate(pred.malignancy = ifelse(pred >= 0.5, "mal","benign")) %>%
       group_by(outcome, pred.malignancy) %>%
       tally()
    outcome pred.malignancy     n
     <fctr>           <chr> <int>
1    benign          benign   434 true negative
2    benign             mal    10 false positive
3 malignant          benign    11 false negative
4 malignant             mal   228 true positive
```

Evaluating the classifier

```
    outcome pred.malignancy     n
     <fctr>           <chr> <int>
1    benign          benign   434 true negative
2    benign             mal    10 false positive
3 malignant          benign    11 false negative
4 malignant             mal   228 true positive
```

```
TPR = TP / (TP + FN)    = 228 / (228 + 11)        = 0.953
FPR = FP / (FP + TN)    = 10 / (10 + 434)         = 0.023
TNR = 1 – FPR                                     = 0.977
PPV = TP / (TP + FP)    = 228/(228 + 10)          = 0.957
Acc = (TP+TN) / (total) = (228 + 434) / (683)     = 0.969
```

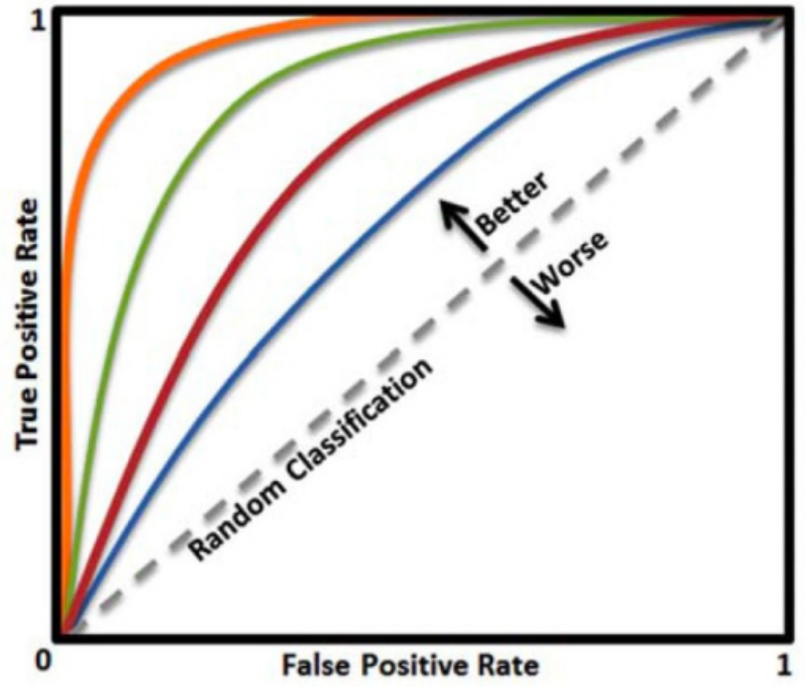
What about for **any possible** cutoff?

Receiver Operating Characteristic (ROC) curves are a common tool to diagnose the ability of a binary classifier

Quantify with metric **AUC**

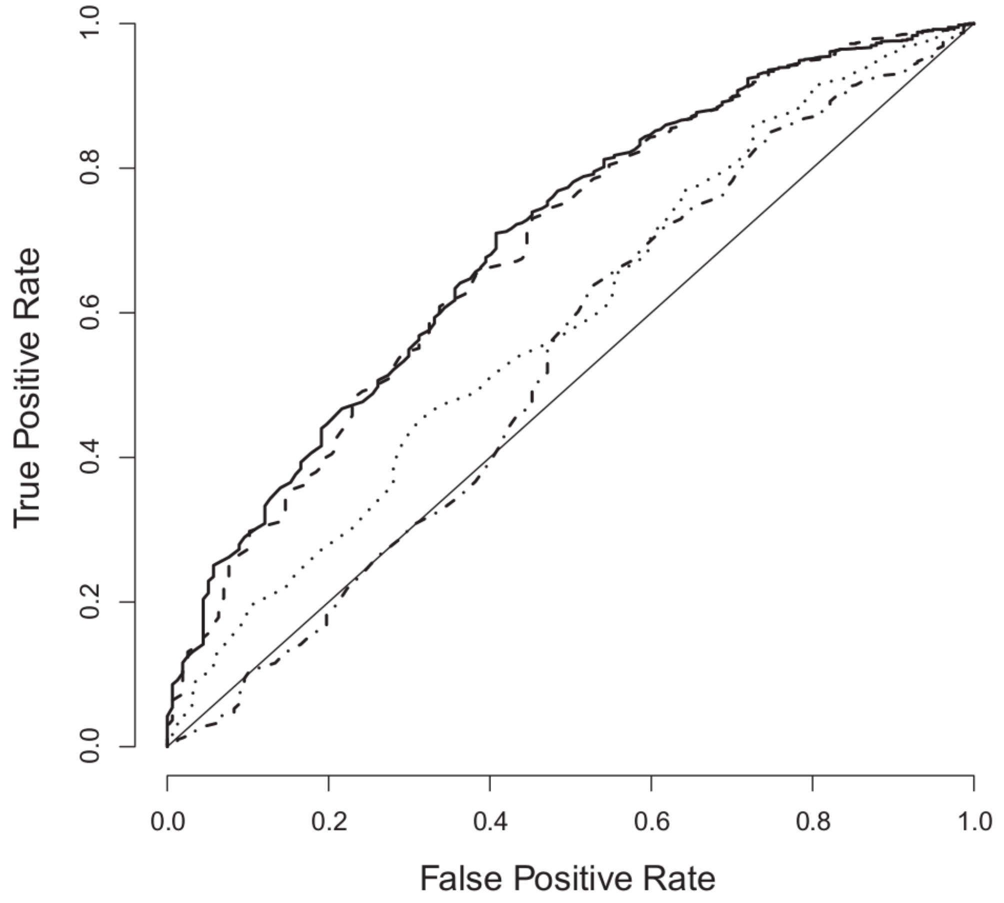
- **A**rea **U**nder the **C**urve (literally)
- 0.5 = random classification
- 1 = perfect classification

TPR = Sensitivity



FPR= 1 - Specificity

Real-life ROC curves



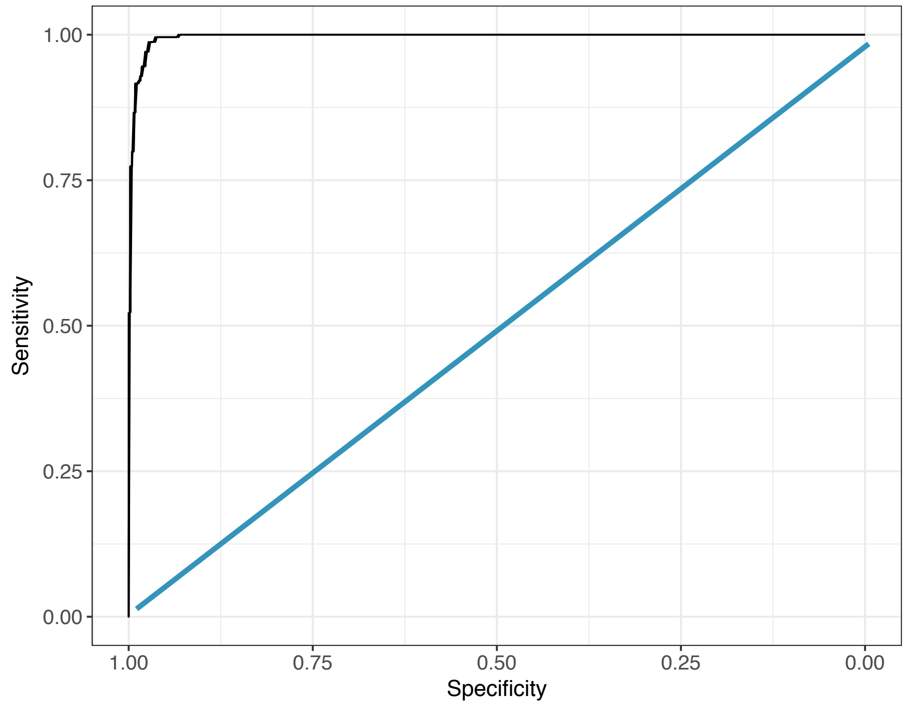
Keller, Mis, Jia, Wilke. Genome Biol. Evol. 4:80-88, 2012

ROC and AUC for our biopsy model

```
> library(pROC) ### You will have to install this package

## the 2nd argument can be either linear.predictors or fitted.values
> roc.object <- roc(biopsy$outcome, model$linear.predictors)

> roc.object$auc
     Area under the curve: 0.9963
```

Visualize the ROC curve

```
> roc.data <- tibble(x = roc.object$specificities,
                     y = roc.object$sensitivities)

> ggplot(roc.data, aes(x = x, y = y)) +
      geom_line() + scale_x_reverse() +
      ylab("Sensitivity") +
      xlab("Specificity")
```



Model selection via AUC

```
> tidy(model)
                   term      estimate  std.error   statistic      p.value
1           (Intercept) -10.103942243 1.17487744 -8.59999681 7.971831e-18
2       clump_thickness   0.535014068 0.14201743  3.76724220 1.650608e-04
3     uniform_cell_size  -0.006279717 0.20907739 -0.03003537 9.760388e-01
4    uniform_cell_shape   0.322706496 0.23060065  1.39941710 1.616879e-01
5         marg_adhesion   0.330636915 0.12345089  2.67828703 7.399977e-03
6  epithelial_cell_size   0.096635417 0.15659236  0.61711452 5.371592e-01
7           bare_nuclei   0.383024572 0.09384327  4.08153469 4.473930e-05
8       bland_chromatin   0.447187920 0.17138238  2.60929928 9.072785e-03
9       normal_nucleoli   0.213030682 0.11287348  1.88734050 5.911454e-02
10              mitoses   0.534835631 0.32877389  1.62675821 1.037885e-01
```

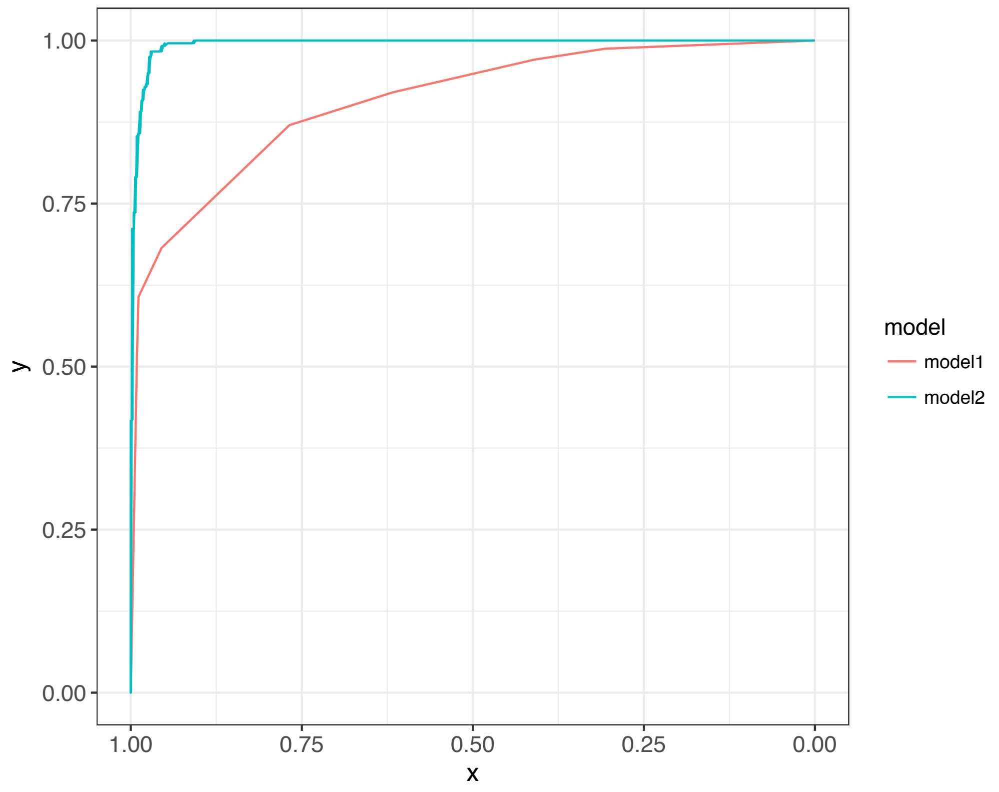
```
> model1 <- glm(outcome ~ clump_thickness, data=biopsy, family=binomial)
> model2 <- glm(outcome ~ clump_thickness + marg_adhesion + bare_nuclei +
                          bland_chromatin, data=biopsy, family=binomial)
```

Model selection via AUC

```
> model1 <- glm(outcome ~ clump_thickness, data=biopsy, family=binomial)
> roc1 <- roc(biopsy$outcome, model1$linear.predictors)
> roc1$auc
      Area under the curve: 0.9089


> model2 <- glm(outcome ~ clump_thickness + marg_adhesion + bare_nuclei +
                            bland_chromatin, data=biopsy, family=binomial)
> roc2 <- roc(biopsy$outcome, model2$linear.predictors)
> roc2$auc
      Area under the curve: 0.9947
```

Directly compare ROC curves

```
> roc1.data <- tibble(x = roc1$specificities,
                      y = roc1$sensitivities,
                      model = "model1")
> roc2.data <- tibble(x = roc2$specificities,
                      y = roc2$sensitivities,
                      model = "model2")

> roc.both <- rbind(roc1.data, roc2.data)

> ggplot(roc.both, aes(x=x,y=y,color=model)) +
       geom_line() + scale_x_reverse()
```



Breathe break

Linear model selection and evaluation

Quantities of **model fit** (how well does my model fit the data?)

- ~~R^2~~
- Likelihood
- Akaike Information Criterion (AIC)
- Bayesian Information Criterion (BIC)

```
> model <- lm(Sepal.Length ~ Petal.Length, data = iris)
> glance(model)
    r.squared adj.r.squared       sigma   statistic         p.value df
1 0.7599546458  0.7583327177 0.407074548 468.5501535 1.038667419e-47  2
       logLik         AIC         BIC    deviance df.residual
1 -77.02021159 160.0404232 169.0723291 24.52503377         148
```

Likelihood

The **likelihood** of a model is the probability of observing your data, given the model's parameters

- $\boldsymbol{P(data|\, parameters)}$

Generally we use LogL (ln likelihood), because likelihoods are very very small

An example likelihood calculation

I flip a coin 500 times and get 380 heads, 120 tails. What is the likelihood of a model with *p=0.5*?

$$P(k\ successes) = \binom{n}{k} p^k q^{(n-k)}$$

$$P(380\ successes \mid p = 0.5) = \binom{380}{500} 0.5^{380} 0.5^{120}$$ = **5.9e-30**

LogL = ln(5.9e-30) = **-74.21**

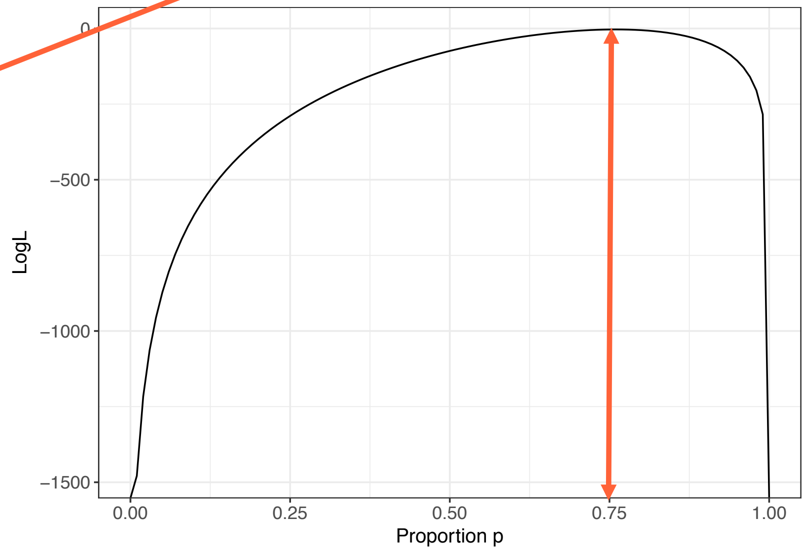
```
> dbinom(380, 500, p=0.5)
[1] 5.9030476e-33

> log(dbinom(380, 500, p=0.5))
[1] -74.209839

> dbinom(380, 500, p=0.5, log=T)
[1] -74.209839
```

Maximum likelihood estimation (**very** simply)

Estimation approach to find the parameter value which **maximizes** the likelihood

```
> all.p <- seq(0, 1, by=0.01) #### 0, 0.01, 0.02,..., 0.99, 1.0
> all.logl <- dbinom(x=380, prob=all.p, size=500, log=T)

> p.logl <- tibble(x = all.p, y = all.logl)
> ggplot(p.logl, aes(x=x,y=y)) +
       geom_line() +
       xlab("Proportion p") +
       ylab("LogL")

> p.logl %>% filter(y == max(y))
      x            y
  <dbl>        <dbl>
1  0.76 -3.176213056
```

The parameter value which maximizes the LogL is the MLE



The likelihood ratio test (LRT)

Hypothesis test to compare fit between two **nested models**

- Parameters of the null model are also in the alternative
- The null is **less** complex. It is a **special case of the alternative**

Uses the chi-squared distribution

- df = (df alternative) – (df null)

$$D = -2\ln\left(\frac{LogL_{null}}{LogL_{alternative}}\right) = 2 \; * [LogL_{alternative} - LogL_{null}]$$

LRT null vs alternative: Which is which?

```
       Null Outcome ~ x1 + x2 + x3

Alternative Outcome ~ x1 + x2 + x3 + x4 + x5
            Outcome ~ x1 + x2 + x3 + 0  +  0
```

Performing a LRT

$$D = -2\ln\left(\frac{LogL_{null}}{LogL_{alternative}}\right)$$
$$= 2 * LogL_{alternative} - LogL_{null}$$

```
> null_model <- lm(Sepal.Length ~ Petal.Length, data = iris)
> tidy(null_model) %>% select(term, estimate)
          term     estimate
1  (Intercept) 4.3066034150
2 Petal.Length 0.4089222774
> glance(null_model) %>% select( adj.r.squared, df, logLik)
  adj.r.squared df       logLik
1  0.7583327177  2 -77.02021159
```

Y = 4.307 + 0.409X

→ The log likelihood of a model with estimated parameters $\boldsymbol{\beta}_0$ = 4.307 and $\boldsymbol{\beta}_1$ = 0.409 is -77.02

```
> alt_model <- lm(Sepal.Length ~ Petal.Length + Species, data = iris)
> glance(alt_model) %>% select( adj.r.squared, df, logLik)
  adj.r.squared df       logLik
1  0.8333687938  4 -48.11637097

#### LRT #####
> D <- 2 * (-48.11637097 - -77.02021159) ### Comes out to 57.80768
> df <- 4 - 2
> 1 - pchisq(D, df)
[1] 2.799982468e-13
```

Evidence for model improvement in the alternative compared to the null.

LRT has very specific utility

Can only compare nested models

```
####### These are not appropriate for LRT #########
> null_model <- lm(Sepal.Length ~ Sepal.Width, data = iris)
> alt_model <- lm(Sepal.Length ~ Petal.Length + Species, data = iris)
```

Can only compare two models

- Not useful if I have 100 models and want to choose the "best" one

Linear model selection and evaluation

Quantities of **model fit** (how well does my model fit the data?)

- ~~R^2~~
- Likelihood
- **Akaike Information Criterion (AIC)**
- **Bayesian Information Criterion (BIC)**

```
> model <- lm(Sepal.Length ~ Petal.Length, data = iris)
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      logLik         AIC         BIC    deviance df.residual
1 -77.02021159 160.0404232 169.0723291 24.52503377         148
```

Comparing non-nested models

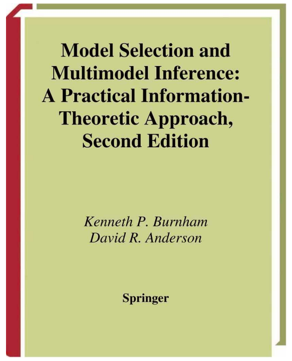
AIC and BIC take *number of parameters* into account to protect against overfitted models

$$AIC = 2 * (k - LogL)$$

$$BIC = k * \log(n) - 2 * LogL$$

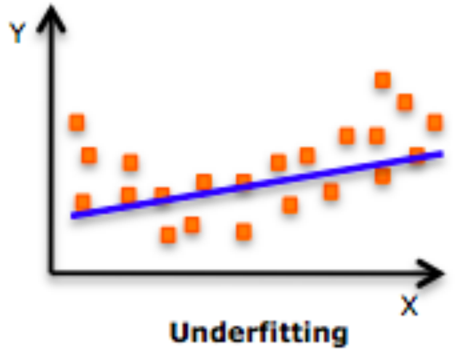
k = number of parameters
n = sample size
BIC penalizes more strongly

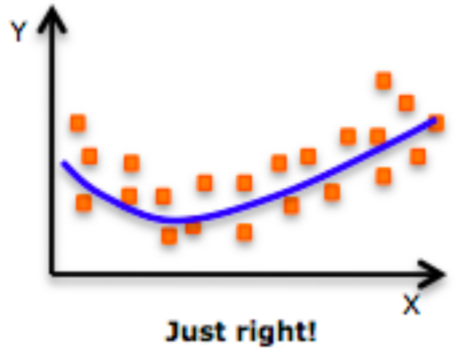
Useful for: Is it worth the overfitting risk to have the additional parameters?

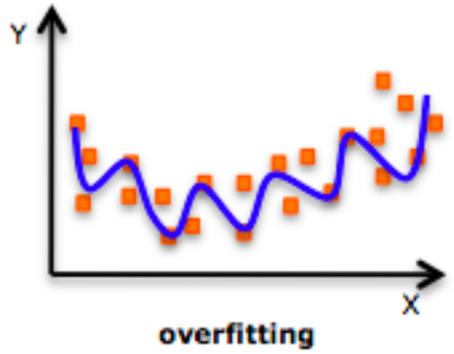

Model Selection and Multimodel Inference: A Practical Information-Theoretic Approach, Second Edition

Kenneth P. Burnham
David R. Anderson

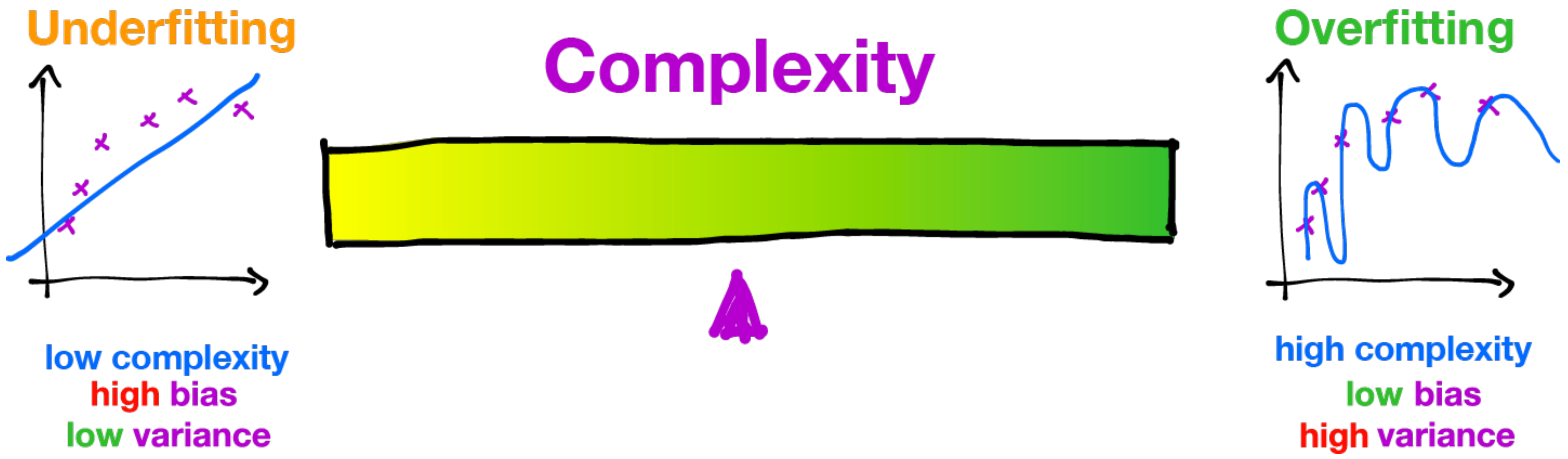
Springer







Bias-variance tradeoff in model fitting



Prefer model with lowest IC ($\Delta IC \sim 2$)

```
> model1 <- lm(Sepal.Length ~ Petal.Length, data = iris)
> glance(model1) %>% select( AIC, BIC)
          AIC         BIC
1 160.0404232 169.0723291

> model2 <- lm(Sepal.Length ~ Petal.Length + Species, data = iris)
> glance(model2) %>% select( AIC, BIC)
          AIC         BIC
1 106.2327419 121.2859184

> model3 <- lm(Sepal.Length ~ Petal.Length * Species, data = iris)
> glance(model3) %>% select( AIC, BIC)
         AIC         BIC
1 106.7673053 127.8417524

> model4 <- lm(Sepal.Length ~ Sepal.Width * Petal.Length * Species, data = iris)
> glance(model4) %>% select( AIC, BIC)
          AIC         BIC
1 80.40596946 119.5442283
```

With AIC, we prefer:

model4 >> model2 ~=model3 >> model1

With BIC, we prefer:

model4 >~ model2 > model3 >>model4

Exhaustive searching in R (one option of millions)

```
> model <- lm(Sepal.Length ~ ., data = iris)

### Selection with AIC
> aic.backwards <- step(model, trace=F)   ## trace=F reduces output vomit
> aic.forwards  <- step(model, trace=F, direction = "forward")

#### Selection with BIC
> bic.backwards <- step(model, trace=F, criterion = "BIC")
```

Exhaustive search results

```
> glance(aic.backwards)
    r.squared adj.r.squared         sigma   statistic          p.value df
1 0.8673122616  0.8627050485 0.3068261031 188.2509525 2.666942494e-61  6
       logLik         AIC         BIC    deviance df.residual
1 -32.55801067 79.11602135 100.1904684 13.55648508         144

> glance(aic.forwards)
    r.squared adj.r.squared         sigma   statistic          p.value df
1 0.8673122616  0.8627050485 0.3068261031 188.2509525 2.666942494e-61  6
       logLik         AIC         BIC    deviance df.residual
1 -32.55801067 79.11602135 100.1904684 13.55648508         144


> glance(bic.backwards)
    r.squared adj.r.squared         sigma   statistic          p.value df
1 0.8673122616  0.8627050485 0.3068261031 188.2509525 2.666942494e-61  6
       logLik         AIC         BIC    deviance df.residual
1 -32.55801067 79.11602135 100.1904684 13.55648508         144
```

Breathe break

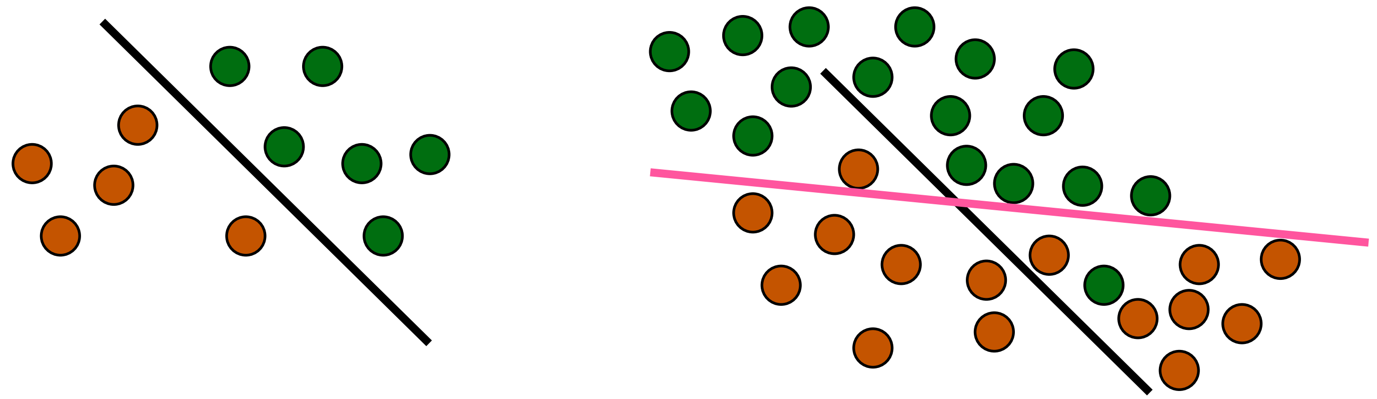
It matters what data you use to build a model

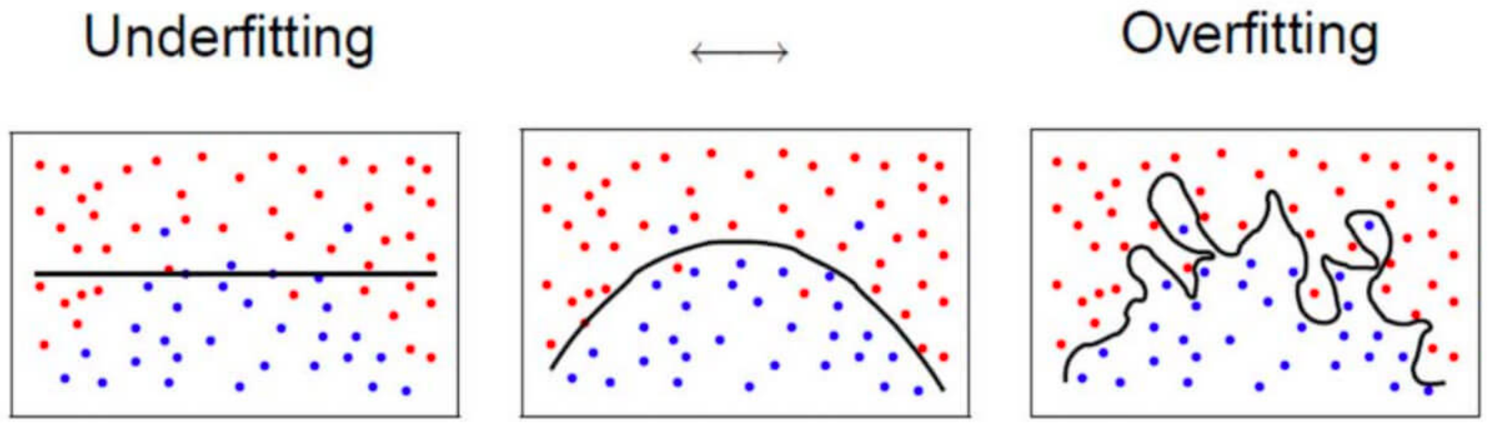
```
> iris %>% sample_frac(0.2) -> iris.sub1
> iris %>% sample_frac(0.2) -> iris.sub2

> m1 <- lm(Sepal.Length ~ Petal.Length, data = iris.sub1)
> glance(m1) %>% select(r.squared)
    r.squared
1 0.8522912784

> m2 <- lm(Sepal.Length ~ Petal.Length, data = iris.sub2)
> glance(m2)
    r.squared
1 0.7443233142

> test.data <- tibble(Petal.Length = 8.7)
```

```
> predict(m1, test.data, interval = "confidence")
    fit         lwr         upr
1 8.174451411 7.791955193 8.556947628
```

```
> predict(m2, test.data, interval = "confidence")
          fit         lwr         upr
1 7.833587103 7.325629373 8.341544834
```

A model is only as good as the data used to **train** it





Model validation strategy

1. Randomly divide data into:
    1. Training data (~60-80%)
    2. Testing data (remaining %)

2. Build model with training data

3. Fit model to test data and assess performance
    1. Categorical response: Accuracy, PPV, TPR, FNR, AUC….
    2. Numeric response: RMSE (root mean square error) = $\sqrt{\frac{1}{n}\sum_i(\hat{y}_i - y_i)^2}$
        1. Has same units as the response variable

First, a single test/train set

```
> iris.train <- iris %>% sample_frac(0.7)
> iris.test <- anti_join(iris, iris.train)


> trained.model <- lm(Sepal.Length ~ Petal.Length, data = iris.train)

### modelr::rmse(model, test.data) ####
> modelr:: rmse(trained.model, iris.test)
[1] 0.4103412

> summary(iris$Sepal.Length)
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max. 
  4.300   5.100   5.800   5.843   6.400   7.900 

> modelr:: rmse(trained.model, iris.train)
[1] 0.4035663
```

The RMSE in predicted Sepal Lengths on the test data is 0.41

RMSE is the same for training data, showing that our models is not biased towards mediocre data.

Test/train for logistic regression

```
> biopsy.train <- biopsy %>% sample_frac(0.7)
> biopsy.test <- anti_join(biopsy, biopsy.train)


> trained.model <- glm(outcome ~ ., data = biopsy.train, family=binomial)

### Mutate the predicted test outcomes into test data
> biopsy.test %>%
       mutate(pred = predict(trained.model, biopsy.test, type="response")) %>%
       select(outcome, pred) -> tested

> head(tested)
    outcome        pred
1    benign 0.006931554
2    benign 0.085382168
3    benign 0.018999048
4    benign 0.003708158
5 malignant 0.999934931
6 malignant 0.602477655
```

Compute various classifier metrics at 0.5 cutoff

```
> tested %>%
      mutate(pred.malignancy = ifelse(pred > 0.5, "mal","benign")) %>%
      group_by(outcome, pred.malignancy) %>%
      tally()
 # Groups:   outcome [?]
    outcome pred.malignancy     n
     <fctr>           <chr> <int>
1    benign          benign    51 true negative
2    benign             mal     4 false positive
3 malignant          benign     4 false negative
4 malignant             mal    63 true positive


  PPV      = TP / (TP + FP)     = 51/(51+ 4)          = 0.927
  Accuracy = (TP+TN) / (total) = (51 + 63) / (122)    = 0.934
```

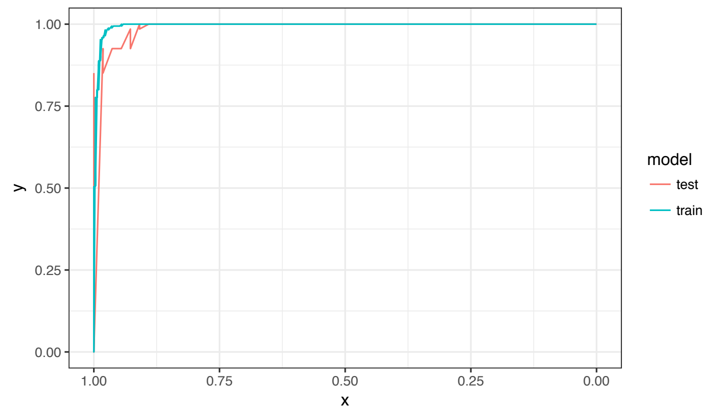
AUC calculations

```
> roc.train <- roc(biopsy.train$outcome, trained.model$linear.predictors)
> roc.train$auc
Area under the curve: 0.996


> test.predictions <- predict(trained.model, biopsy.test)
> roc.test <- roc(biopsy.test$outcome, test.predictions)
> roc.test$auc
Area under the curve: 0.9929
```

Consistency between training and testing data!

ROC curves for training and testing

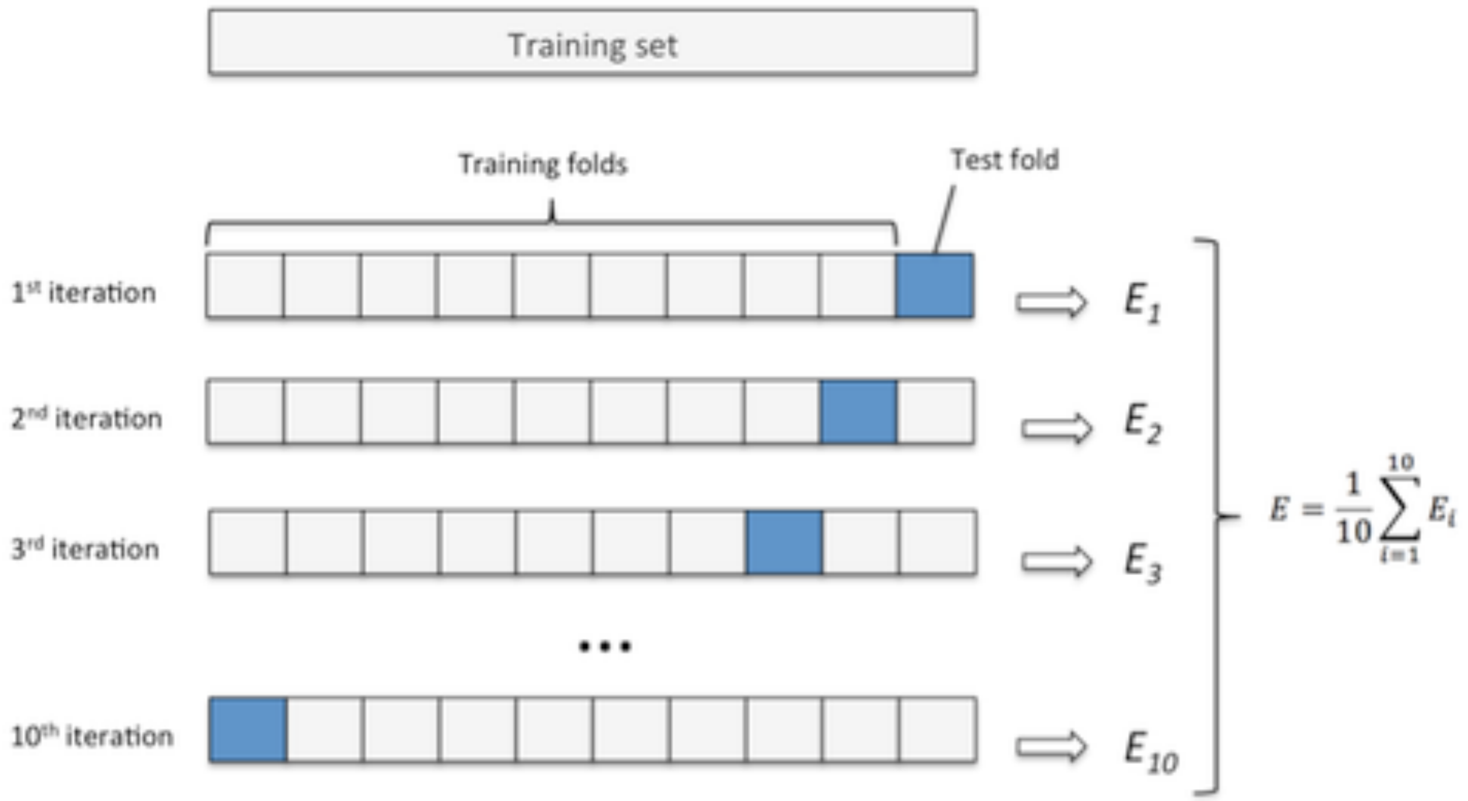
```
> roc.data.train <- tibble(x = roc.train$specificities,
                           y = roc.train$sensitivities,
                                  model = "train")
> roc.data.test <- tibble(x = roc.test$specificities,
                          y = roc.test$sensitivities,
                                 model = "test")

> rbind(roc.data.train, roc.data.test) %>%
      ggplot(aes(x=x, y=y, group=model, color=model)) +
      geom_line() +
      scale_x_reverse()
```



K-fold cross validation is common and powerful

1. Split data randomly into *k* evenly spaced chunks
    1. K=10 is a good choice, K=5 for smaller datasets
2. Take first chunk as testing, and remaining chunks as training
3. Evaluate on test data
4. Repeat k times, so each chunk is used once as a test set

K-fold cross validation



Special case is Leave-one-out cross validation (LOOCV), where k=n