# 2001-353-w06b-p-Resamp-PredictionErrorEstimates-FeatureSelection

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# 23 February, 2023

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#### 6.1.2.1 Reading, Homeworks, Projects, SemProjects

- Readings for next class:
  - For Today, ISLR7 Beyond Linear Models, (R4DS22-25)
  - For next Tuesday ISLR8 and DL08/DL09
- Laboratory Exercises:
  - LE3 due on Today
  - LE4 given out Tommorrow
- Office Hours: (Class Canvas Calendar for Zoom Link)
  - Wednesdays @ 4:00 PM to 5:00 PM
  - Saturdays @ 3:00 PM to 4:00 PM
  - Office Hours are on Zoom, and recorded
- Semester Projects
  - Office Hours for SemProjs: Mondays at 4pm on Zoom
  - DSCI 453 Students Biweekly Updates Due
    - \* Update # is Due \*\* \*\*
  - DSCI 453 Students
    - \* Next Report Out # is Due \*\* \*\*
  - All DSCI 353/353M/453, E1453/2453 Students:

- \* Peer Grading of Report Out #1 is Due \*\* \*\*
- Exams
  - \* MidTerm: Thursday March 9th, in class or remote, 11:30 12:45 PM
    - · CWRU Spring Break is March 13th to March 17, so NO CLASS
  - \* Final: Thursday May 4th, 2023, 12:00PM 3:00PM, Nord 356 or remote

#### 6.1.2.2 Textbooks

#### 6.1.2.2.1 Introduction to R and Data Science

- For students new to R, Coding, Inferential Statistics
  - Peng: R Programming for Data Science
  - Peng: Exploratory Data Analysis with R
  - OIS = Diez, Barr, Çetinkaya-Runde: Open Intro Stat v4

#### 6.1.2.3 Tidyverse Cheatsheets, Functions and Reading Your Code

- Look at the Tidyverse Cheatsheet
  - Tidyverse For Beginners Cheatsheet
    - \* In the Git/20s-dsci353-353m-453-prof/3-readings/3-CheatSheets/ folder
  - Data Wrangling with dplyr and tidyr Cheatsheet ]

Tidyverse Functions & Conventions

- The pipe operator %>%
- Use dplyr::filter() to subset data row-wise.
- Use dplyr::arrange() to sort the observations in a data frame
- Use dplyr::mutate() to update or create new columns of a data frame
- Use dplyr::summarize() to turn many observations into a single data point
- Use dplyr::arrange() to change the ordering of the rows of a data frame
- These can be combined using dplyr::group\_by()
  - which lets you perform operations "by group".
- The %in% matches conditions provided by a vector using the c() function
- The **forcats** package has tidyverse functions
  - for factors (categorical variables)
- The readr package has tidyverse functions
  - to read\_..., melt\_... col\_..., parse\_... data and objects

Reading Your Code: Whenever you see

- The assignment operator  $\leftarrow$ , think "gets"
- The pipe operator, %>%, think "then"

# **6.1.2.4** Syllabus

#### 6.1.2.5 ISLR Chapter 5 Resampling Methods: Prediction Error Estimates

- Having procedures to evaluate different statistical methods is essential
  - Such as using Training and Testing Datasets
    - \* So that we can determine the prediction accuracy
    - \* Or the prediction error

Resampling Methods also do the same thing

- Such as Cross-validation
- Bootstrap

Day:Date	Foundation	Practicum	Readings(optional)	Duc(optional)
w01a:Tu:1/17/23	Markov Cluster	R, Rstudio IDE, Git	B ( 1 1 1 1 1 )	(LE0)
w01b:Th:1/19/23	Stat. Learning, Ap-	Bash, Git. Class Repo	ISLR1,2 (R4DS-1-3)	(DDO)
, 10, 20	proach	2001, 010, 01000 100,00	1021(1;2 (1(12:0 1 0)	
w02a:Tu:1/24/23	Lin. Regr. Bias-Var.	SemProjs; Regr. Ovrvw	ISLR3,(R4DS-4-6)	(LE0:Due) LE1
w02b:Th:1/26/23	Train/Test, Bias vs. Vari.	Tidyverse Review	DL01 DL02 (R4DS-7.8)	(EEG.E GO) EEG
w02Pr:Fr:1/27/23	ADD DROP	DEADLINE		453 Update 1
w03a:Tu:1/31/23	Logistic Regr. Classif	Pred. Analytics, Regr.	DL03.ISLR4	
w03b:Th:2/2/23	LDA/QDA	ggPlot2, Code Expect.	DL04, DL05	LE1:Due, LE2
w03:Sa:2/4/23		00		LE1:Due
w04a:Tu:2/7/23	Resample Cross-Valid.	ggplot	ISLR5	
w04b:Th:2/9/23	DL, ML Overview	Multilevel Mod.	ISLR6 (R4DS9-16)	
w04Pr:Fr:2/10/23				453 Update 2
w05a:Tu:2/14/23	Resampling: Bootstrap	Bootstrap Mixed Effects	DL2R1, DL06,07	LE2:Due, LE3
w05b:Th:2/16/23	Subset Selec., Shrink.	Dim. Red. PCA	DLwR2	BEZ.Buc, EE.
w05Pr:Fr:2/17/23				453 Rep. Out 1
w06a:Tu:2/21/23	ML with NNs	ggplot, clustering	DLwR3	
w06b:Th:2/23/23	Beyond Linear Modls	Feature Select., Caret	ISLR7 (R4DS22-25)	LE3:Due, LE4
w06Pr:Fr:2/24/23			(	453 Update 3
w07a:Tu:2/28/23	Dec. Trees, Rand. Forest	Tidy Modeling	ISLR8, DL08,09	
w07b:Th:3/2/23	MidTerm Review, SVM	SVM, SVR, ROC	ISLR9 (R4DS26-30)	Peer Review 1
w08a:Tu:3/7/23	ML Overview	, Keras/TF2, Torch	ISLR10	
w08b:Th:3/9/23	MIDTERM EXAM	, Reras/112, Toren	DL10,11	LE4:Due LE5
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 $Table\ 1:\ DSCI353-353M-453\ Weekly\ Syllabus.\ R4DS-x.y,\ OISx.y,\ ISLRx.y,\ DLGBx.y\ refers\ to\ chapters\ and\ sections\ assigned\ as\ reading\ in\ our\ textbooks.\ DLx\ are\ deep\ learning\ articles.$ 

Figure 1: IT Fundamentals: Applied Data Science with R, Syllabus

• Leave-one-out cross-validation

In addition there are other metrics of statistical significance

We've seen

- $R^2$  and  $adj.R^2$
- p-values for null hypothesis testing

There are also  $C_p$  statistic, AIC and BIC and others

- Malloy's  $C_p$  statistic
- Akaike Information Criteria, AIC
- Bayesian Information Criteria, BIC

# 6.1.2.6 Training and Testing for Prediction Error Determination

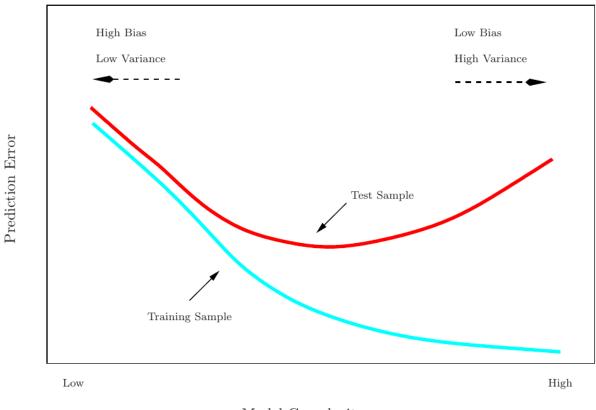
• Training vs. Testing Error

# Training Error versus Test error

- Recall the distinction between the *test error* and the *training error*:
- The *test error* is the average error that results from using a statistical learning method to predict the response on a new observation, one that was not used in training the method.
- In contrast, the *training error* can be easily calculated by applying the statistical learning method to the observations used in its training.
- But the training error rate often is quite different from the test error rate, and in particular the former can dramatically underestimate the latter.

Training vs. Testing Performance

# Training- versus Test-Set Performance



Model Complexity

# 6.1.2.7 Cross-validation and Bootstrap

 $\bullet\,$  Cross-validation and Bootstrap

# Cross-validation and the Bootstrap

- In the section we discuss two *resampling* methods: cross-validation and the bootstrap.
- These methods refit a model of interest to samples formed from the training set, in order to obtain additional information about the fitted model.
- For example, they provide estimates of test-set prediction error, and the standard deviation and bias of our parameter estimates

# 6.1.2.8 Other Prediction Error Estimates

• Other Prediction Error Estimates

# More on prediction-error estimates

- Best solution: a large designated test set. Often not available
- Some methods make a mathematical adjustment to the training error rate in order to estimate the test error rate. These include the Cp statistic, AIC and BIC. They are discussed elsewhere in this course
- Here we instead consider a class of methods that estimate the test error by *holding out* a subset of the training observations from the fitting process, and then applying the statistical learning method to those held out observations

#### 6.1.3 ISLR6 Linear Model Selection and Regularization

#### 6.1.3.1 Feature or Variable Selection

• These are all parts of the general topic of Feature Selection

In machine learning and statistics, feature selection,

- also known as variable selection,
  - attribute selection or variable subset selection,
- is the process of selecting a subset of relevant features
  - (variables, predictors) for use in model construction.

Feature selection techniques are used for three reasons:

- simplification of models to make them easier to interpret by researchers/users,
- shorter training times,
- enhanced generalization by reducing overfitting
  - (formally, reduction of variance)

The central premise when using a feature selection technique is

- that the data contains many features that are either redundant or irrelevant,
- and can thus be removed without incurring much loss of information.

Redundant or irrelevant features are two distinct notions,

- since one relevant feature may be redundant
- in the presence of another relevant feature
  - with which it is strongly correlated.

Feature selection techniques should be distinguished from feature extraction.

- Feature extraction creates new features from functions of the original features,
- whereas feature selection returns a subset of the features.

Feature selection techniques are often used in domains

- where there are many features
- and comparatively few samples (or data points).

Archetypal cases for the application of feature selection include

- the analysis of written texts and
- DNA microarray data,

where there are many thousands of features,

• and a few tens to hundreds of samples.

### 6.1.3.2 Prediction Error Estimates and Optimality Criteria

• And Optimality Criteria

Three common ones are the following

- Malloy's  $C_p$  Statistic
- Aikake Information Criteria
- Bayesian Information Criteria

# 6.1.3.2.1 Malloy's $C_p$ Statistic

- In statistics, Mallows's  $C_n$ ,
  - named for Colin Lingwood Mallows,

- is used to assess the fit of a regression model
  - \* that has been estimated using ordinary least squares.

It is applied in the context of model selection,

- where a number of predictor variables are available for predicting some outcome,
  - and the goal is to find the best model involving a subset of these predictors.
- A small value of  $C_p$  means that the model is relatively precise.

Mallows's  $C_p$  has been shown to be equivalent

- to Akaike information criterion
  - in the special case of Gaussian linear regression.

#### 6.1.3.2.2 Aikake Information Criteria

- The Akaike information criterion (AIC)
  - is a measure of the relative quality of statistical models
    - \* for a given set of data.
    - \* based on Shannon's information theory and information entropy

Given a collection of models for the data,

- AIC estimates the quality of each model,
  - relative to each of the other models.
- Hence, AIC provides a means for model selection.

AIC is founded on information theory:

- it offers a relative estimate of the information lost
  - when a given model is used to represent the process that generates the data.
- In doing so, it deals with the trade-off between
  - the goodness of fit of the model
  - and the complexity of the model.
- The Akaike information criterion (AIC)
  - is a measure of the relative quality of statistical models
  - for a given set of data.
- Given a collection of models for the data,
  - AIC estimates the quality of each model,
  - relative to each of the other models.
- Again, AIC provides a means for model selection.

AIC does not provide a test of a model

• in the sense of testing a null hypothesis; i.e.

AIC can tell nothing about the quality of the model in an absolute sense.

- If all the candidate models fit poorly,
- AIC will not give any warning of that.

### 6.1.3.2.3 Bayesian Information Criteria

- In statistics, the Bayesian information criterion (BIC)
  - or Schwarz criterion (also SBC, SBIC)
  - is a criterion for model selection
    - \* among a finite set of models;
    - \* the model with the lowest BIC is preferred.

It is based, in part, on the likelihood function

• and it is closely related to the Akaike information criterion (AIC).

When fitting models,

- it is possible to increase the likelihood by adding parameters,
- but doing so may result in overfitting.

Both BIC and AIC resolve this problem

- by introducing a penalty term for the number of parameters in the model;
- the penalty term is larger in BIC than in AIC.

The BIC was developed by Gideon E. Schwarz

- and published in a 1978 paper,
- where he gave a Bayesian argument for adopting it.

#### 6.1.3.3 Cites

- Gareth James, Daniela Witten, Trevor Hastie, and Robert Tibshirani. An Introduction to Statistical Learning: With Applications in R. 1st ed. 2013, Corr. 5th printing 2015 edition. Springer Texts in Statistics. New York: Springer, 2013.
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