1.0 Intro to Machine Learning

Intro to Machine Learning

A form of AI that enables a system to learn from data. -IBM

- Supervised learning
  - Prediction of a given output using other variables in the data set
  - Used for tasks involving the prediction of a given output (target, Y variable) using predictor variables (features, X variable)
  - Finds patterns that can be applied to an analytic process
- Unsupervised learning
  - Performs analysis without target variable
  - Used when the problem requires a lot of unlabled data

X and Y Terminology

- X-Variable
  - Predictor variable
  - Independent variable
  - Attribute
  - Feature
- Y-Variable
  - Target variable
  - Dependent variable
  - Response
  - Outcome Measurement

Basic Processes

ML Steps

- Define and understand purpose
  - What is the problem statement?
- Get data
  - May involve random sampling
- Clean and process data
  - Ensure data is accurate
  - DS spend 70-80% of time here

- Partition data for generlizability
  - Generalizeability of our algorithm
  - Fits our past data and predicts the future
- Reduce data
- Specify task
- Choose the techniques
- Iterative implementation and tuning

Partioning Data for Generalizability

- Split data into training and testing data
- Training data to train algos for choosing the final model
- Testing data for model's performance
- Split recommendations (training%/testing%):
  - 60/40, 70/30, 80/20
  - Splitting can be done in R by sampling portions of data
    - Be sure to use consistent seeds
- Overfitting
  - Doesn't allow us to get a good assessment of training performance
  - Typically with higher traing% splits
- Underfitting
  - Having too little test data to assess our model

Partioning Data in R

Data: Wisconsin Breast Cancer

```r
# Read in Wisconsin breast cancer data
wis.df <- read.csv("Data Sets/1.2-wisc_bc_data.csv")
```

Partition data the easy way

- Knowing the count of observations and feeding those row numbers into separate variables
- Querying dataframes syntax:
  - `dataframe.df[rows,columns]`
  - Leaving either argument blank returns all values
  - Below we grab specific rows, and all columns because it's blank

```r
train <- wis.df[1:469,]
test <- wis.df[470:569,]
```

Partition data with sampling

Create Training Data

> `sample` takes a sample of the specified size from the elements of x using either with or without replacement.

```
sample(x, size, replace = FALSE, prob = NULL)
```

`dim` has a method for data.frames, which returns the lengths of the row.names attribute of x and of x (as the numbers of rows and columns respectively) - Assumption about what's happening because prof didn't explain: - Sample the rownames column - … With the size of the length(`dim`) of the first column `[1]` - … Multiplied by 0.7 to get 70%

Create the training data, add it to the dataset

```r
train2.row <- sample(rownames(wis.df),dim(wis.df)[1]*0.7)
# Add training data to the data set
train2 <- wis.df[train2.row,]

# Optional: view train2 to see number of observations
#str(train2)
```

Create Test Data

- Use setdiff to get the rows from the first argument that aren't in the second argument
  - In this case the rows in our original df that aren't in the training data

The elements of setdiff(x,y) are those elements in x but not in y.

```r
test2.row <- setdiff(rownames(wis.df),train2.row)
# Add training data to the data set
test2 <- wis.df[test2.row,]
```

Model Performance Evaluation

Overfitting

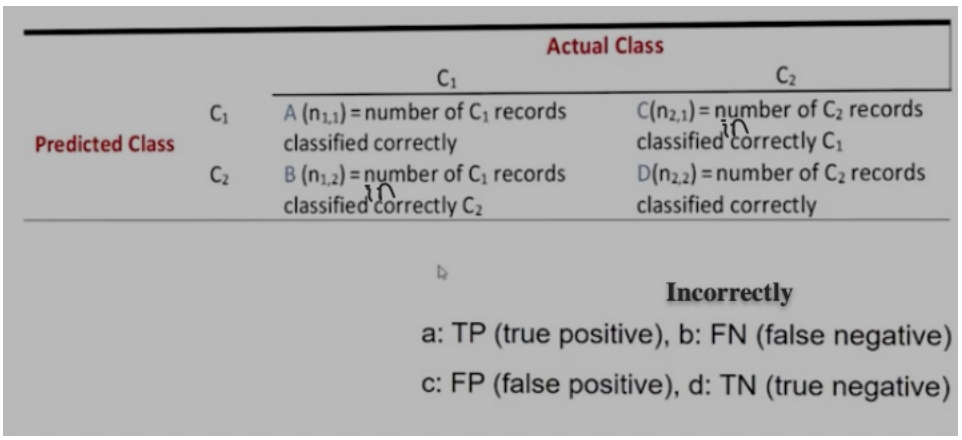
- Causes
  - Too many predictors
  - Too many parameters
  - Trying many different models
    - May wind up picking one that just happens to fit your training data the best
- Consequence: the deployed model won't work as well with brand new data ### Measuring Predictive Error
- Used for predictive numerical values where the outcome is numerical, e.g. house prices
- Not the same as goodness-of-fit, standard error (r^2) (difference between actual and predicted Y, or "error")
  - This merely compares the model to the data it was trained with
  - We are interested in the model's ability to predict new records
    - How do we do that? Witchcraft mostly.
    - Also by validating the error of the training model against the test data

Measure Classifier Performance

For categorical data - Evaluation - Measure the classifier accuracy by dividing the proportion of correct predictions by the total number of predictions - The error being misclassification - Goals of evaluation models - Attempting to understand how model performance will extrapolate to future cases - A natural criterion - Actual class values - Predicted class values - Estimated probablity of the prediction

Confusion/Misclassification Matrix

- A matrix showing the results between actual and predicted classifications
- Errors (false positive and false negative) are found in $(n_{1,2})$ and $(n_{2,1)})$
- Can be used to find the error rate and accuracy



		Actual Class	
		C_1	C_2
Predicted Class	C_1	A $(n_{1,1})$ = number of C_1 records classified correctly	C$(n_{2,1})$ = number of C_2 records classified in correctly C_1
	C_2	B $(n_{1,2})$ = number of C_1 records classified in correctly C_2	D$(n_{2,2})$ = number of C_2 records classified correctly

Incorrectly

a: TP (true positive), b: FN (false negative)

c: FP (false positive), d: TN (true negative)

Figure 1: Confusion Matrix

- Note: $(n_{1,2})$ and $(n_{2,1)})$ should read "incorrectly"

Calculating Error Rate and Accuracy *Error Rate:* $ErrorRate = \frac{FP+FN}{TP+TN+TP+TN} = 1 - accuracy$

Accuracy: $Accuracy = 1 - ErrorRate$

Limitations of Accuracy Given two groups: - Group 1 observed 9990 times - Group 2 observed 10 times

- If a model predicted all 10,000 observations to be group 1, the accuracy would be 9990/10000 = 99.9%
  - This is misleading because the model did not detect any members of group 2

Cutoff Table

- If the cutoff is 0.5 as indicated by the dividing line, every 1 on the right side and 0 on the left is an error

Use the `confusionMatrix()` function from the `caret` package. > The caret package (short for Classification And REgression Training) is a set of functions that attempt to streamline the process for creating predictive models.

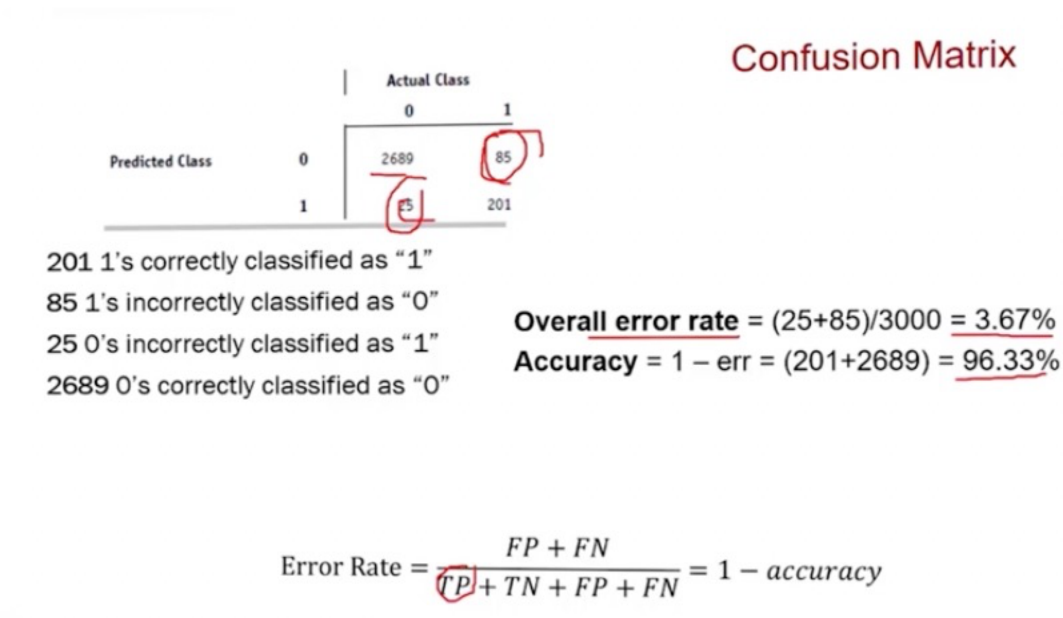
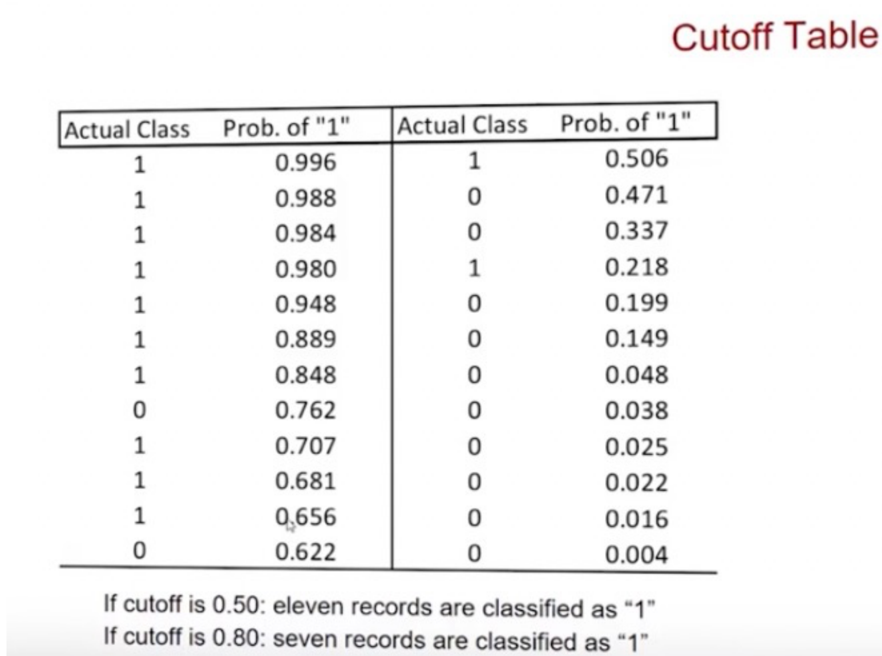


Figure 2: Confusion Matrix Example



Cutoff Table

Actual Class	Prob. of "1"	Actual Class	Prob. of "1"
1	0.996	1	0.506
1	0.988	0	0.471
1	0.984	0	0.337
1	0.980	1	0.218
1	0.948	0	0.199
1	0.889	0	0.149
1	0.848	0	0.048
0	0.762	0	0.038
1	0.707	0	0.025
1	0.681	0	0.022
1	0.656	0	0.016
0	0.622	0	0.004

If cutoff is 0.50: eleven records are classified as "1"
If cutoff is 0.80: seven records are classified as "1"

Figure 3: Cutoff Table

[confusionMatrix] Calculates a cross-tabulation of observed and predicted classes with associated statistics.

- `confusionMatrix(data, reference)`
  - data: the predicted classification
    - In this example we compute the prediction with an if/else and store it as column "Predicted" in "owner"
      - If the probability is greater than 0.5, classify as owner. Otherwise, classify as nonowner.
    - We need to be sure to cast this new column as a factor so it can be used by `confusionMatrix()`
      - Use `as.factor()`
  - reference: the "actual" classifications

```
#install.packages("caret", repos = "http://cran.us.r-project.org")
```

```
library(caret)
```

```
owner <- read.csv("Data Sets/1.3-owner.csv")

# Create Predicted classification
owner$Predicted <- ifelse(owner$Probability>0.5, 'owner', 'nonowner')

# Build confusion matrix casting Predicted as a factor
confusionMatrix(as.factor(owner$Predicted), as.factor(owner$Class))
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction nonowner owner
##   nonowner       10     1
##   owner           2    11
##
##                Accuracy : 0.875
##                  95% CI : (0.6764, 0.9734)
##     No Information Rate : 0.5
##     P-Value [Acc > NIR] : 0.0001386
##
##                   Kappa : 0.75
##
##  Mcnemar's Test P-Value : 1.0000000
##
##             Sensitivity : 0.8333
##             Specificity : 0.9167
##          Pos Pred Value : 0.9091
##          Neg Pred Value : 0.8462
##              Prevalence : 0.5000
##          Detection Rate : 0.4167
##    Detection Prevalence : 0.4583
##       Balanced Accuracy : 0.8750
##
##        'Positive' Class : nonowner
##
```

```r
str(owner)
```

```
## 'data.frame':    24 obs. of  3 variables:
##  $ Class      : chr  "owner" "owner" "owner" "owner" ...
##  $ Probability: num  0.996 0.988 0.984 0.98 0.948 ...
##  $ Predicted  : chr  "owner" "owner" "owner" "owner" ...
```

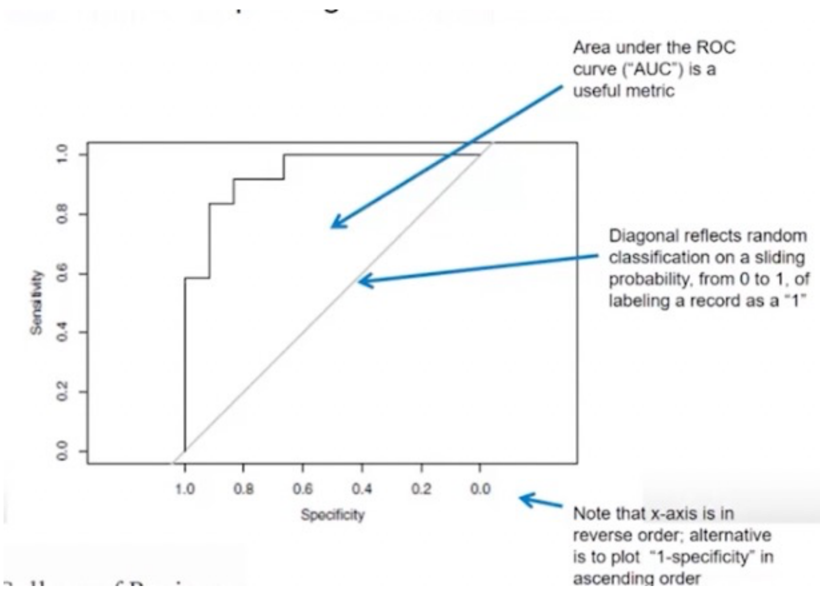
Other Criteria

Beyond Accuracy

- Useful classifiers balance between predictions that are overly conservative or aggressive
- Sensitivity vs. specificity
    - Sensitivity
        * The ability to detect the important class members correctly
        * E.g. the % of C1 members classified correctly $Sensitivity = \frac{a}{a+b}$
    - Specificity
        * The ability to rule out other members correctly
        * E.g. the % of C2 members classified correctly $Specificity = \frac{d}{c+d}$
- Precision and recall

Receiver Operating Characteristic (ROC) Curve

- A method for plotting sensitivity and specificity cutoff values from 1 to 0
    - The x-axis (specificity) is reversed from 1 to 0, you could also write it ascending as 1 - specificity
- Better performance would be in the top left corner
- Area under the curve (AOC) is a useful metric for judging classifier
    - 1 is a perfect classification
    - .9-1 is excellent
    - .8-.9 is good
    - .7-.8 is fair
    - .6-.7 is poor
    - .5-.6 is failure



ROC in R Install the `pROC` package > This is the main function of the pROC package. It builds a ROC curve and returns a "roc" object

- Use `roc(response, predictor)` to get a dataframe of ROC points
  - Response is the "true class"
    - In our case `owner$Class`
  - Predictor is the predicted value of each observation, must match the length of response
    - In our case `owner$Probability`
- Use `auc()` to obtain the area under the curve value

```
#install.packages("pROC")
```

```
library(pROC)
```

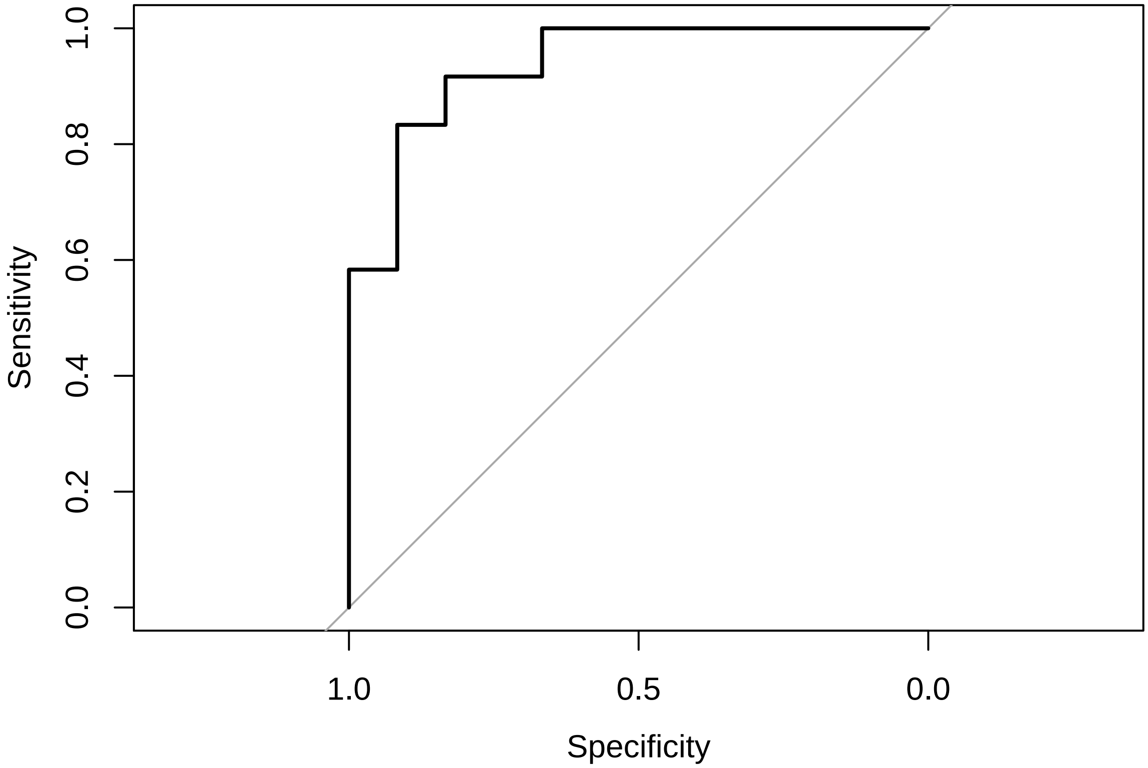
```
# Read in data
owner <- read.csv("Data Sets/1.3-owner.csv")

# Create roc object and store in r
r <- roc(owner$Class, owner$Probability)
```

```
## Setting levels: control = nonowner, case = owner
```

```
## Setting direction: controls < cases
```

```
# Plot the roc
plot.roc(r)
```




```r
# Obtain the AUC value
auc(r)
```

```
## Area under the curve: 0.9375
```