DATA SOCIETY®

Week 7 Day 1 - Intro to classification

"One should look for what is and not what he thinks should be."
-Albert Einstein.

Module completion checklist

Objective	Complete
Summarize the steps & application of kNN	
Clean and transform the data to run kNN	
Define cross validation and how and when it is used	
Implement the kNN algorithm on the training data without cross-validation	
Identify performance metrics for classification algorithms	
Evaluate the optimal number of nearest neighbors to use using cross-validation	
Evaluate performance of optimized kNN model	
Apply the knn and evalute its performance on the CMP dataset	

Directory settings

• First, let's make sure to set our directories correctly, this way, we will not have to worry about this throughout the course

```
# Set `main dir` to the location of your `hhs-r` folder (for Mac/Linux).
main_dir = "~/Desktop/hhs-r-2020"
# Set `main dir` to the location of your `hhs-r` folder (for Windows).
main_dir = "C:/Users/[username]/Desktop/hhs-r-2020"
# Make `data_dir` from the `main_dir` and
# remainder of the path to data directory.
data_dir = paste0(main_dir, "/data")
# Make `plots_dir` from the `main_dir` and
# remainder of the path to plots directory.
plot_dir = paste0(main_dir, "/plots")
```

Loading packages

Let's load the packages we will be using:

```
#install.packages("ROCR")
#install.packages("e1071")
library(e1071)
library(caret)
library(ROCR)
```

kNN: what is it?

- The k-nearest-neighbors (kNN) algorithm is a **supervised learning** algorithm.
- It is primarily used for **Classification**.
- It takes a bunch of labeled points and uses them to learn how to label other points.

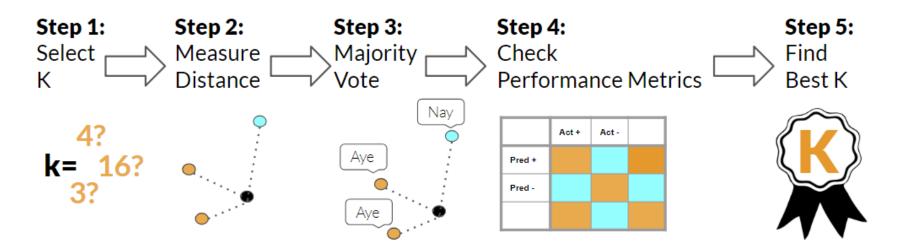
Classification vs. regression

	Classification	Regression
Target	Discrete, usually binary	Continuous
variable		
Types	Binary, Multi-Class	Linear
Algorithms	Decision trees, random forest, logistic regression, K-	Linear regression, regression trees, time-
	nearest neighbors	series regression

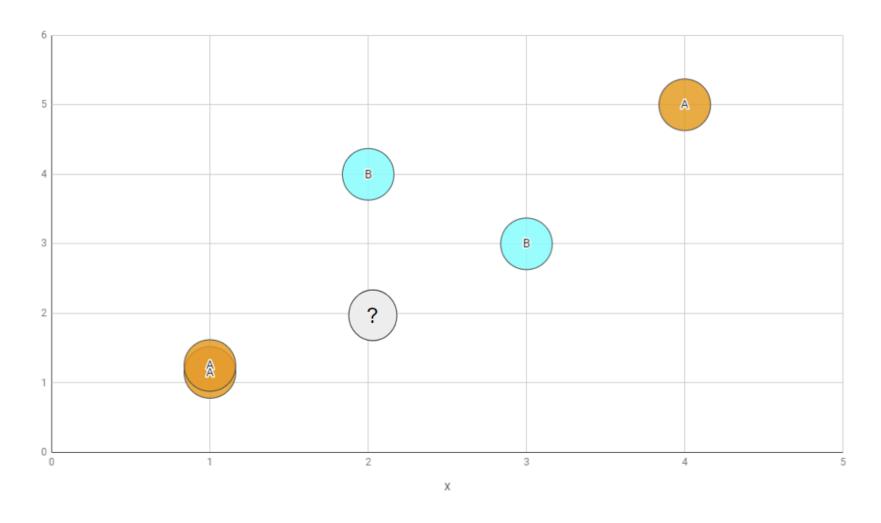
Classification: assigning to groups

Question to answer	Real world example
What is this object like?	Selecting similar products at the lowest prices
Who is this person like?	Anticipating behavior or preferences of a person based on her similarities
	with others
What category is this in?	Anticipate if your customer is pregnant, remodeling, just got married, etc.
What is the probability that	Determine the probabilitythat a piece of equipment will fail, determine the
something is in a given category?	probability that someone will buy your product

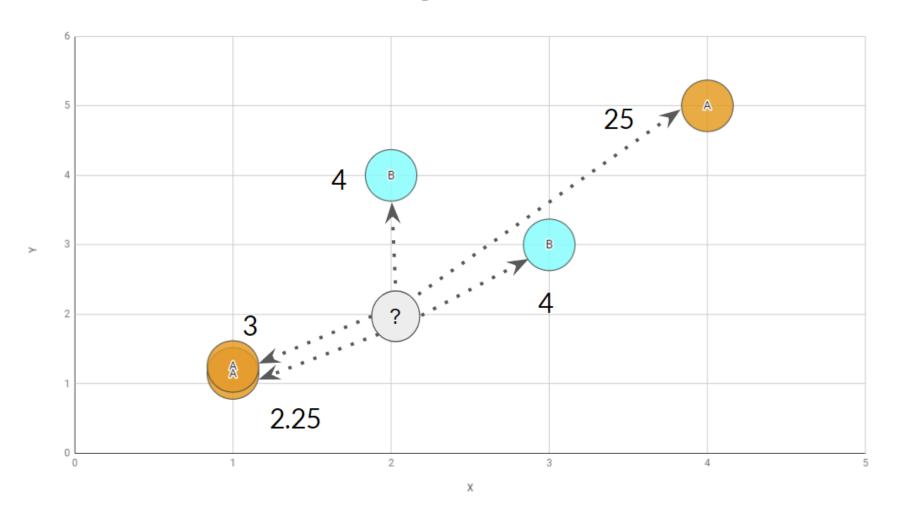
Steps of kNN



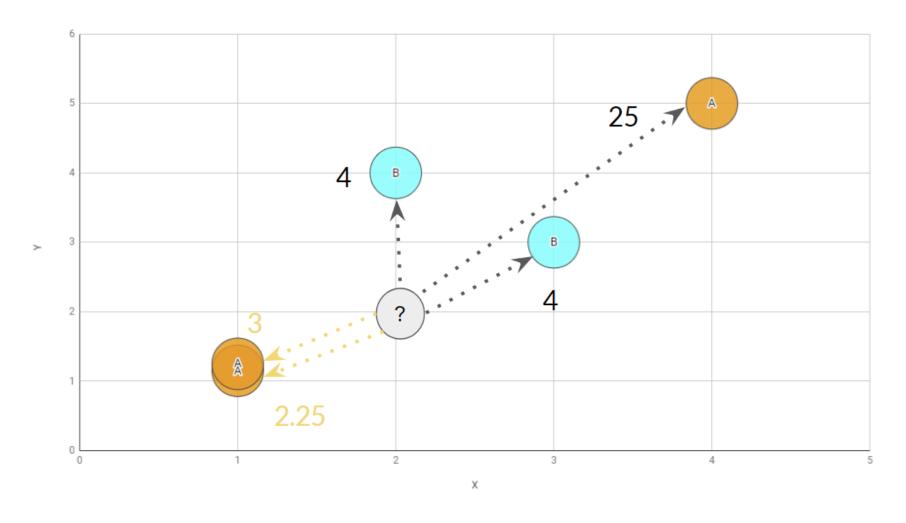
k-Nearest Neighbors: set up



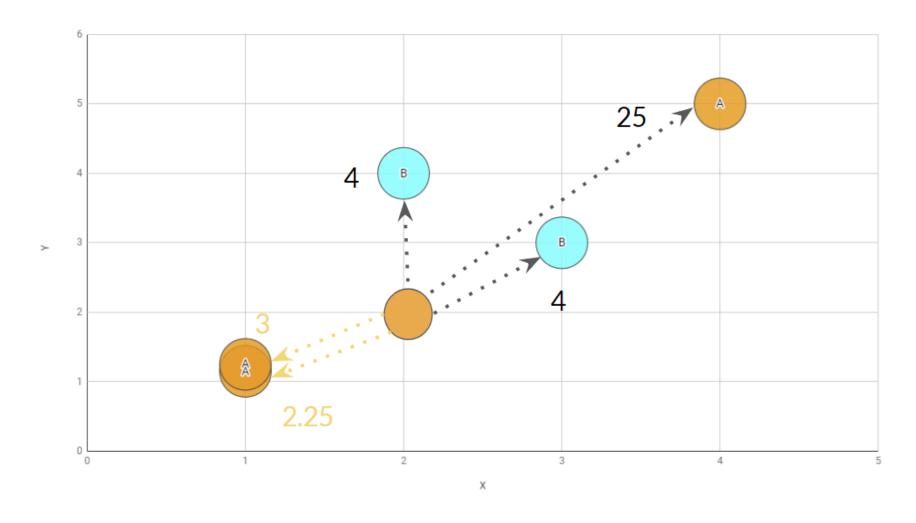
k-Nearest Neighbors: measure



k-Nearest Neighbors: 2-NN for majority vote



k-Nearest Neighbors: label point



Knowledge check 1



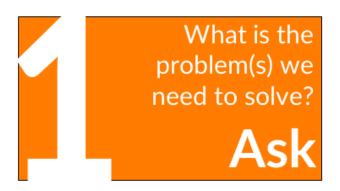
Exercise 1



Module completion checklist

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kNN: example one - business case



A new medicine is out and is being questioned regarding the effect it has on heart rate; the **medication will increase heart rate** and the researchers are now sure it does not vary by gender specifically, but want to **classify gender** for new patients using temperature and heart rate.

We have been given a sample of participants who took the medication for a study. We have:

- Gender,
- Heart rate, and
- Temperature of each participant

We want to use kNN to predict the **classification** of each data point to either Male or Female.

Directory Settings

- In order to maximize the efficiency of your workflow, you may want to encode your directory structure into variables
- Let the main dir be the variable corresponding to your hhs-r-2020 folder

```
# Set `main dir` to the location of your `hhs-r-2020` folder (for Mac/Linux).
main_dir = "~/Desktop/hhs-r-2020"
# Set `main_dir` to the location of your `hhs-r-2020` folder (for Windows).
main_dir = "C:/Users/[username]/Desktop/hhs-r-2020"

# Make `data_dir` from the `main_dir` and remainder of the path to data directory.
data_dir = paste0 (main_dir, "/data")
# Make `plots_dir` from the `main_dir` and remainder of the path to plots directory.
plot_dir = paste0 (main_dir, "/plots")

# Set directory to data_dir.
setwd(data_dir)
```

Load the dataset

We will now load the dataset that consists of three variables:

- Gender
- Temperature
- Heart Rate

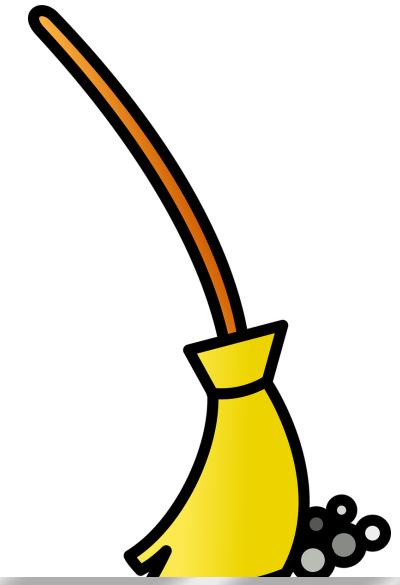
```
setwd(data_dir)
temp_heart = read.csv("temp_heart_rate.csv",
TRUE)
head(temp_heart)
```



Data cleaning steps for kNN

Like the other algorithms we have covered, there are a few steps to take before jumping into splitting the data and training the model:

- 1. Check for NAs
- 2. Scale the predictors
- 3. Make sure the target is labeled



The data at first glance

```
Female Male 0.5 0.5
```

temp heart[,1])) # <- denotes the variable that is being evaluated

Check for NAs

Check for NAs

- 1. What is the percentage of NAs in our dataset?
- 2. We need to divide the sum of all entries that are NA by the sum of those that aren't.

```
# Let's find all NAs in the dataset.
is_NA = is.na(temp_heart)

# Are there NAs in the dataset?
sum(is_NA) / sum(!is_NA)
```

```
[1] 0
```

Doesn't look like we have to deal with NAs in this dataset.

Scaling the predictors

Scale the predictors

- 1. Let's create a new object, temp heart scaled, where we will scale the predictors only
- 2. We then add the target variable Gender to the new scaled dataset

```
# Scale the predictors, transform the data to a data frame so
# that we can add gender back in
temp_heart_scaled = as.data.frame(sapply(temp_heart[,2:3],scale))

# Make sure to add gender back to the scaled data set
gender = temp_heart[,1]
temp_heart_scaled$Gender = gender

# Inspect scaled values
head(temp_heart_scaled)
```

```
Body.Temp Heart.Rate Gender
1 -2.658586 -0.53263914 Male
2 -2.113020 -0.39103773 Male
3 -1.840237 0.03376649 Male
4 -1.703845 0.88337493 Male
5 -1.567454 -0.10783492 Male
6 -1.567454 0.17536790 Male
```

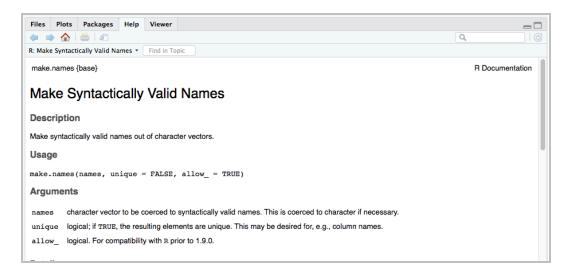
Defining a target variable

- kNN will have either a binary target or a multi-class target
- In the case of the heart rate dataset we are dealing with a **binary** target
- Our target variable here is Gender which has two levels Male and Female
- If we have a *continuous* variable as a target, we manipulate it to become **binary** / **multi-class**
- We will address this later today when we introduce kNN on the CMP dataset

Prepare for prediction: labeling the target

- In preparing for prediction, the levels of the target variable will be used as variable names for prediction
- To do this, we use the function make.names

```
?make.names
make.names(names) #<- character vector to be
coerced syntactically to valid names</pre>
```



Prepare for prediction: labeling the target

We need to make sure the levels are valid variable names using the functionmake.names

```
# Setting levels for both training and test data
levels(temp_heart_scaled$Gender) =
   make.names(levels(factor(temp_heart_scaled$Gender)))

levels(temp_heart_scaled$Gender) =
   make.names(levels(factor(temp_heart_scaled$Gender)))
```

Cross-validation: Remember this?

Train

- This is the data that you train your model
 on
- Usually about 70% of your dataset
- Use a larger portion of the data to train so that the model gets a large enough sample of the population
- If there is not a large population on the whole, cross-validation techniques can be implemented

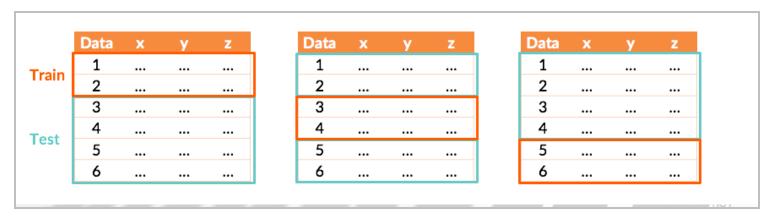
Test

- This is the data that you test your model
 on
- Usually about 30% of your dataset
- Use a smaller portion to test your trained model on
- If cross-validation is implemented, small test sets will be held out multiple times

Cross-validation: n-fold

Earlier, we split into test and train once. Here is the idea now:

- 1. Split the dataset into several subsets ("n" number of subsets) of equal size
- 2. Use each subset as the test data set and use the rest of the data as the training dataset
- 3. Repeat the process for every subset you create



Train & test: small scale before n-fold

- Before we actually use n-fold cross-validation:
 - We split our data into a train and test set
 - We run kNN initially on the training data

kNN: modeling with caret & train

 We will use the kNN function implemented through the caret package, using the train function

- x: The predictors from the training set
- y: The target from the training set
- method: This will be knn here
- trControl: We will use this to define cv parameters
- metric: The parameter we will use to select the optimal model

```
Packages Help
R: Fit Predictive Models over Different Tuning Parameters * Find in Topic
                                                                                                            R Documentation
Fit Predictive Models over Different Tuning Parameters
Description
This function sets up a grid of tuning parameters for a number of classification and regression routines, fits each model and calculates a resampling based
Usage
train(x, ...)
## Default S3 method:
train(x, y, method = "rf", preProcess = NULL, ...,
  weights = NULL, metric = ifelse(is.factor(y), "Accuracy", "RMSE"),
  maximize = ifelse(metric %in% c("RMSE", "logLoss", "MAE"), FALSE, TRUE),
 trControl = trainControl(), tuneGrid = NULL,
  tuneLength = ifelse(trControl$method == "none", 1, 3))
## S3 method for class 'formula'
train(form, data, ..., weights, subset, na.action = na.fail,
 contrasts = NULL)
## S3 method for class 'recipe'
train(x, data, method = "rf", ...,
 metric = ifelse(is.factor(y_dat), "Accuracy", "RMSE"),
  maximize = ifelse(metric %in% c("RMSE", "logLoss", "MAE"), FALSE, TRUE),
  trControl = trainControl(), tuneGrid = NULL,
  tuneLength = ifelse(trControl$method == "none", 1, 3))
```

kNN: train the model

- Let us run kNN on the training data, using train
- Notice that we do not include the trControl parameter

```
k-Nearest Neighbors
92 samples
 2 predictor
 2 classes: 'Female', 'Male'
No pre-processing
Resampling: Bootstrapped (25 reps)
Summary of sample sizes: 92, 92, 92, 92, 92, 92,
Resampling results across tuning parameters:
 k Accuracy
                Kappa
  5 0.5800895 0.1761705
  7 0.5901166 0.1985280
  9 0.5865995 0.1907089
Accuracy was used to select the optimal model
using the largest value.
The final value used for the model was k = 7.
```

kNN: predict on test

 Now we will take our trained model and predict on the test set

- What we get is a vector of predicted values
- This is helpful because we have the actual values for this sample
- We can calculate the accuracy of our model using the actual values compared to the predicted values

```
Male
                 Male
                        Male
                                     Male
 [1] Male
                              Male
Female Female Male
                 Female
                                     Female
[11] Male Male
                 Female Female Male
Female Female Male
[21] Male
           Male
                 Male
                        Male
                              Male
                                     Male
Female Male
           Male
                   Female
[31] Female Male
                 Female Female Female
Female Female
Levels: Female Male
```

Knowledge check 2



Exercise 2



Module completion checklist

Objective	Complete
Summarize the steps & application of kNN	/
Clean and transform the data to run kNN	/
Define cross validation and how and when it is used	/
Implement the kNN algorithm on the training data without cross-validation	V
Identify performance metrics for classification algorithms	
Evaluate the optimal number of nearest neighbors to use using cross-validation	
Evaluate performance of optimized kNN model	
Apply the knn and evalute its performance on the CMP dataset	

Classification: assessing performance

- We have reviewed how to measure error when using regression
- Because our outcome variable is binary
 we have a different way of measuring error
 than when the outcome variable was
 continous

- The following terms are very important to measure performance of a classification algorithm
 - Confusion matrix

Confusion matrix: What is it?

Confusion matrix is what we use to assist us in measuring error

We will use it to calculate Accuracy, Misclassification rate, True positive rate, False positive rate and Specificity

	Female	Male	Predicted Totals:
Predicted	True Positive	False Positive	Total Predicted
Female	(TP)	(FP)	Positive
Predicted	False	True Negative	Total Predicted
Male	Negative (FN)	(TN)	Negative
Actual Totals:	Total Positives	Total Negatives	Total

Confusion matrix: for temp heart data

Let's look at the confusion matrix for the temp_heart_test predictions - using 7 NN

	Female	Male	Predicted Totals:
Predicted Female	13 True Positive (TP)	7 False Positive (FP)	20
Predicted Male	6 False Negative (FN)	12 True Negative (TN)	18
Actual Totals:	19	19	38

Confusion matrix: accuracy

Accuracy: overall, how often is the classifier correct?

TP + TN / total = (13 + 12) / 38

	Female	Male	Predicted Totals:
Predicted Female	13 True Positive (TP)	7 False Positive (FP)	20
Predicted Male	6 False Negative (FN)	12 True Negative (TN)	18
Actual Totals:	19	19	38

Confusion matrix: misclassification rate

Misclassification rate (error rate): overall, how often is the classifier wrong?

$$FP + FN / total = (7 + 6) / 38$$

	Female	Male	Predicted Totals:
Predicted Female	13 True Positive (TP)	7 False Positive (FP)	20
Predicted Male	6 False Negative (FN)	12 True Negative (TN)	18
Actual Totals:	19	19	38

Confusion matrix: true positive rate

True positive rate (Sensitivity): how often does it predict yes?

TP / actual yes = **13** / **20**

	Female	Male	Predicted Totals:
Predicted Female	13 True Positive (TP)	7 False Positive (FP)	20
Predicted Male	6 False Negative (FN)	12 True Negative (TN)	18
Actual Totals:	19	19	38

Confusion matrix: false positive rate

False positive rate: when it's actually no, how often does it predict yes?

FP / actual no = **7** / 19

	Female	Male	Predicted Totals:
Predicted Female	13 True Positive (TP)	7 False Positive (FP)	20
Predicted Male	6 False Negative (FN)	12 True Negative (TN)	18
Actual Totals:	19	19	38

Confusion matrix: specificity

True Negative Rate (Specificity): when it's actually no, how often does it predict no?

TN / actual no = **12** / **19**

	Female	Male	Predicted Totals:
Predicted Female	13 True Positive (TP)	7 False Positive (FP)	20
Predicted Male	6 False Negative (FN)	12 True Negative (TN)	18
Actual Totals:	19	19	38

Confusion matrix: model fit for knn

```
k-Nearest Neighbors
92 samples
 2 predictor
 2 classes: 'Female', 'Male'
No pre-processing
Resampling: Bootstrapped (25 reps)
Summary of sample sizes: 92, 92, 92, 92, 92, 92,
Resampling results across tuning parameters:
  k Accuracy
               Kappa
  5 0.5800895 0.1761705
  7 0.5901166 0.1985280
   0.5865995 0.1907089
Accuracy was used to select the optimal model
using the largest value.
The final value used for the model was k = 7.
```

The output of the model says that the number of **k=7** was determined by optimizing for **accuracy** within the **training data set**

i.e. the algorithm tried different values of **k** to see how k impacted **accuracy** and chose the k with the **highest** accuracy.

The algorithm is using an internal confusion matrix.

Confusion matrix: in R

- Now that we know the metrics behind the madness, let's execute the code to build a confusion matrix in R that we can see.
- We use a function confusionMatrix from the caret package

```
Plots Packages Help
R: Create a confusion matrix . Find in Topic
confusionMatrix {caret}
                                                                                                       R Documentation
Create a confusion matrix
Description
Calculates a cross-tabulation of observed and predicted classes with associated statistics
Usage
confusionMatrix(data, ...)
## Default S3 method:
confusionMatrix(data, reference, positive = NULL,
  dnn = c("Prediction", "Reference"), prevalence = NULL,
  mode = "sens spec", ...)
## S3 method for class 'table'
confusionMatrix(data, positive = NULL, prevalence = NULL,
  mode = "sens_spec", ...)
Arguments
data
              a factor of predicted classes (for the default method) or an object of class table.
              options to be passed to table. NOTE: do not include dnn here
             a factor of classes to be used as the true results
```

Confusion matrix: calculate in R

Now we calculate the confusion matrix in R

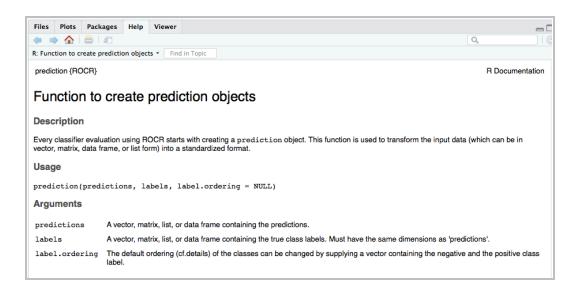
```
Confusion Matrix and Statistics
         Reference
Prediction Female Male
   Female
             10 10
   Male
              Accuracy: 0.5
                95% CI: (0.3338, 0.6662)
   No Information Rate: 0.5
   P-Value [Acc > NIR] : 0.5643
                 Kappa: 0
Mcnemar's Test P-Value: 1.0000
           Sensitivity: 0.4737
           Specificity: 0.5263
        Pos Pred Value: 0.5000
        Neg Pred Value: 0.5000
            Prevalence: 0.5000
        Detection Rate: 0.2368
  Detection Prevalence: 0.4737
     Balanced Accuracy: 0.5000
      'Positive' Class : Female
```

Performance of our kNN model

Now, let's evaluate our model using the ROC curve:

 We use the function prediction from the ROCR package to create a prediction object

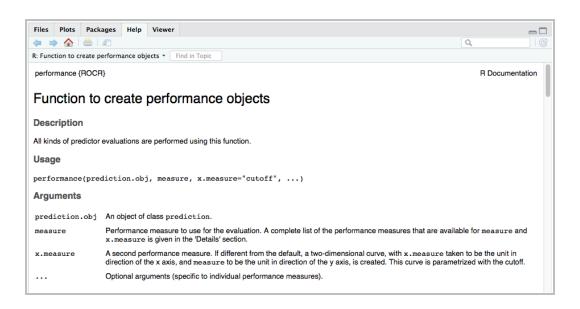
- predictions: the vector of class labels predicted by the kNN model
- labels: the vector of true class labels



Performance of our kNN model

We can now use the function performance from the ROCR package for model evaluation

- prediction.obj: the object we just created using prediction
- measure: a performance measure, in this case, either "tpr" or "auc"
- x.measure: a second performance measure; for ROC curve, use "fpr"



Knowledge check 3



Exercise 3



Module completion checklist

Objective	Complete
Summarize the steps & application of kNN	✓
Clean and transform the data to run kNN	V
Define cross validation and how and when it is used	V
Implement the kNN algorithm on the training data without cross-validation	V
Identify performance metrics for classification algorithms	/
Evaluate the optimal number of nearest neighbors to use using cross-validation	
Evaluate performance of optimized kNN model	
Apply the knn and evalute its performance on the CMP dataset	

1. We have now:

- i. Run kNN on our training data
- ii. Reviewed performance metrics for classification algorithms
- iii. Built a confusion matrix for the predicted model

2. We will now:

- i. Use cross-validation and re-run the model on the training data
- ii. Find what our optimal k value is
- iii. Evaluate the new predictions

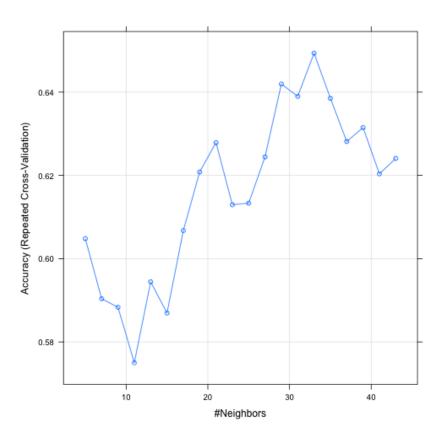
- We will use the train function again, but this time we will bring in the trainControl parameter
- This allows us to choose repeatedcy as the method parameter

- method: use cross-validation
- repeats: repeat cross-validation 3 times
- classProbs: give us the probabilities for each class

Run the model on the training data

Look at the results

```
knn fit cv
k-Nearest Neighbors
92 samples
 2 predictor
 2 classes: 'Female', 'Male'
No pre-processing
Resampling: Cross-Validated (10 fold, repeated 3 times)
Summary of sample sizes: 84, 83, 83, 83, 82, 83, ...
Resampling results across tuning parameters:
 k Accuracy Kappa
   5 0.5333333 0.06538226
   7 0.5412963 0.07970085
  39 0.6233333 0.24725393
  41 0.6165741 0.23475116
  43 0.6256481 0.25133563
Accuracy was used to select the optimal model using the largest value.
The final value used for the model was k = 43.
```



Using the optimized model to predict

- We can use the model we just built to predict on the test set
- It is optimized because of the crossvalidation and will use the optimized k which is k=43
- Although it is an optimized model, it does not mean it will perform better than our previous model, it is just more accurate

```
test_pred_cv = predict(knn_fit_cv,newdata =
temp_heart_test)
```

```
#Get the confusion matrix to see accuracy value and other parameter values confusionMatrix(test_pred_cv, temp_heart_test$Gender)

Confusion Matrix and Statistics

Reference
Prediction Female Male
Female 8 6
Male 11 13

Accuracy: 0.5526
95% CI: (0.383, 0.7138)
...
'Positive' Class: Female
```

KNN pros and cons

PROs

- easy to use
- can easily handle multiple categories
- there are many options to adjust (which features to use, measurement metric, etc)

CONS

- There are many options to adjust
- The correct distance metric is important
- Can be slow with large amounts of data
- Because it is LAZY, memorizes and uses every data point when calculating kNN

Module completion checklist

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Summarize the steps & application of kNN	/
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Implement the kNN algorithm on the training data without cross-validation	V
Identify performance metrics for classification algorithms	/
Evaluate the optimal number of nearest neighbors to use using cross-validation	V
Evaluate performance of optimized kNN model	/
Apply the knn and evalute its performance on the CMP dataset	

kNN on CMP

- We are all familiar with the CMP dataset by now
- Let's start with data pre-processing
 - scale the data
 - impute NAs using the function we built earlier
 - return a cleaned dataset
- We will then have to convert our target variable Yield from continuous to categorical so that we can use a classification algorithm, kNN

kNN on CMP: data pre-processing

```
# Impute NAs in CMP dataset
CMP_NA_impute = ImputeNAsWithMean(CMP_scale)

# rename it as CMP_cleaned
CMP_cleaned = CMP_NA_impute
```

kNN on CMP: converting Yield

- We covered this early on, when we learned ifelse
- Now we see why we would need to convert a variable from continous to categorical
- This is useful, as you now can see how you could use a classification algorithm with a continuous predictor

```
# What are the summary stats of `Yield`?
summary(CMP_cleaned$Yield)
```

```
Min. 1st Qu. Median Mean 3rd Qu. Max. -2.6692 -0.7716 -0.1119 0.0000 0.7035 3.3394
```

```
# Median
summary(CMP_cleaned$Yield)[3]
```

```
Median -0.1119022
```

- Now, we use the median to separate
 Yield into
 - High yield
 - Low yield

```
[1] Low yield High yield High yield High yield High yield High yield Levels: High yield Low yield
```

kNN: train model using cv

Split the data into train and test

Name the levels of the target variable Yield

```
# Make sure to name the levels
levels(CMP_train$Yield) =
  make.names(levels(factor(CMP_train$Yield)))

levels(CMP_test$Yield) =
  make.names(levels(factor(CMP_test$Yield)))
```

kNN: train model using cv

- Set the parameters for trainControl
- Train the model
- Name the model CMP_[algorithm_name]
- We will be comparing models at the end of the 8 weeks

```
CMP knn
k-Nearest Neighbors
124 samples
 57 predictors
  2 classes: 'High.yield', 'Low.yield'
No pre-processing
Resampling: Cross-Validated (10 fold, repeated 3
times)
Summary of sample sizes: 111, 112, 111, 111,
112, 112, ...
Resampling results across tuning parameters:
                Sens
                            Spec
   5 0.8977986 0.7904762 0.8142857
     0.8969482 0.7984127 0.7880952
  15 0.8984505 0.7880952 0.7730159
  43 0.8380197 0.6325397 0.7769841
ROC was used to select the optimal model using
the largest value.
The final value used for the model was k = 15.
```

kNN: predict

Now let's predict on the test set

```
knnPredict = predict(CMP_knn,newdata = CMP_test
)
```

```
#Get the confusion matrix to see accuracy value and other parameter values confusionMatrix(knnPredict, CMP_test$Yield)

Confusion Matrix and Statistics

Reference
Prediction High.yield Low.yield
High.yield 16 12
Low.yield 10 14

Accuracy: 0.5769
'Positive' Class: High.yield
```

Knowledge check 4



Exercise 4



Module completion checklist

Objective	Complete
Summarize the steps & application of kNN	/
Clean and transform the data to run kNN	/
Define cross validation and how and when it is used	/
Implement the kNN algorithm on the training data without cross-validation	V
Identify performance metrics for classification algorithms	/
Evaluate the optimal number of nearest neighbors to use using cross-validation	V
Evaluate performance of optimized kNN model	/
Apply the knn and evalute its performance on the CMP dataset	V

This completes our module **Congratulations!**