Chapter 1

The Pursuit of Prediction

1.1 Map Data as Guestimates

On an early September day in 2013, the staff of Fairbanks International Airport had an unusual encounter: TSA agents intercepted a motorist headed for the airport. This was not just any routine traffic stop — it was on the tarmac of an airfield. A motorist unwittingly drove passed marked signs and lights, venturing down a taxiway and eventually across an active runway on the way to the airport car park (Cole (2013), Koosner (2013)). Later that same month, yet another motorist made the same mistake. What is the connection? Both incidents were the result of faulty driving directions from an iPhone app. Needless to say, the airport blocked the entrance to the tarmac and filed complaints with Apple.

Incidents like these are not uncommon. In fact, competing apps like Waze have led drivers into danger, whether its impassable snow covered roads (Kraus (2019)) or into the path of a wildfire (Wagstaff (2017)). Part of the problem lies in the maintaining an up-to-date record of the built environment. Imagine that the address of every building, condition and speed limits of every road, status of traffic, among other real-time conditions need to be available for any user to use at a moment's. It is a massive challenge that has led companies to acquire other companies to improve data quality (Trenholm (2013)). Sometimes, companies will even use sensitive user data to fill data gaps (Panzarino (2018)). Keeping up-to-date data is a problem of scale – it is simply too hard for humans to manually curate and keep information up to date for literally all of existence.

Machine learning can help.

Everyday, we already rely on high frequency and high resolution data to make even the smallest of decisions, yet we do so often without realizing that much of the data are filled with approximations produced by predictive models. This is the new paradigm of artificial intelligence that has taken the tech sector by storm and its predictive power has been increasingly seen in the service of social and public good. In recent memory, Microsoft illustrated that machine learning algorithms can perform a mapping task that would normally require years for a team of humans to perform. Computer scientists trained a pair of algorithms to identify building footprints. One set of neural network algorithms were trained on five million satellite imagery tiles to identify pixels that belong to buildings, then an additional filter converted pixels into building polygons. (Microsoft (2018)) In other words, one model examines images that contain buildings and non-buildings and predicts which pixels are likely be part of a building. Since there may be some rogue pixels making the building footprint jagged, a second algorithm converts pixels into polygons that resemble realistic building footprints. The methodology achieved a precision of 99.3% and recall of 93.5% — it is quite accurate and scalable. The algorithm was then set loose on satellite imagery for the entirety of the United States, depositing its findings into the first comprehensive national building database containing 125,192,184 building footprints (Wallace, Watkins, and Schwartz (2018)). A complete inventory of the state of the built environment has never been available at this level of resolution and coverage, and could one day support real-time decision

making. When faced with a hurricane, emergency services could have access to a more up-to-date inventory of all structures in the path of destruction, enabling more accurate damage estimates and more informed mitigation strategies. Local governments can make better zoning decisions so cities can evolve intelligently. And perhaps such a database could support address canvasing for the US census.

What if algorithm can provide help distill a mass of data into a simple, more useful form. The economy, for example, is comprised of an extraordinarily large number of variables. Some are related, others are not. When faced with thousands of economic variables, a human analyst may be biased towards what they are familiar or their world perspective. A machine learning algorithm, in contrast, will seek out variables that have the greatest signal for predicting a measure of interest. This is what the U.S. Bureau of Economic Analysis (BEA) has experimented with in recent memory. The agency, which is responsible for estimating the Gross Domestic Product (GDP), is faced with a constant scheduling tango with their data sources – some data are available in time for their advance estimate of GDP and others are not. When data are not available in time, economically-motivated projections carry the estimates forward until when there is an opportunity to incorporate the "gold copy" data. The risk of projection is the chance that it does not reflect the gold copy when it is available, leading to revisions in economic estimates – a source of anxiety for economists and financial analysts. To reduce revisions to service sector estimates, BEA has developed an experimental approach that relies on *ensembles* of machine learning algorithms, such as *Random Forests* and *Regularized Regression*, to sift through thousands of alternative economic variables and predict economic growth before data is available. This strategy has been shown that predictions can reduce revisions to economic estimates by billions of dollars (Chen et al. (Forthcoming)), which in turn can mitigate unnecessary market responses to revisions. Similar prediction strategies have been applied by tech companies to optimize their resources. Uber, for example, trained a Long-Short Term Memory (LSTM) algorithm to forecast ridership when faced with extreme events such as sports events and holidays. By improving their short-range forecasts across their platform, they can better optimize resource allocation to meet customer demand and manage budgets more efficiently (Laptev, Smyl, and Santhosh Shanmugam (Forthcoming)).

The pursuit of prediction has driven computer scientists and statisticians to constantly develop new strategies that maximize predictive accuracy. In fact, each type of machine learning algorithm works best under different circumstances, whether it's the type of data or the use case. Let's revisit the seemingly simple case of classification. Below, we plot three distinct scenarios for a two-class classification problem : simple linear boundary, non-linear, and discontinuous. A *logistic regression* is a natural fit for a linear boundary given its root in linear regression. While it is the champion of parameter estimation, logistic regression is ill-fit for more complex relationships. Non-parametric techniques are far more flexible and can mold the decision boundary to the counters of the data. This gain in accuracy comes at the cost of interpretability. For example, *K-nearest neighbors* (kNN) performs classification by looking at neighborhoods of observations. Given a training sample, each record in the test sample is predicted using the most common label for the k closest known records. In essence, kNN is driven by a majority or plurality vote from neighboring records. Alternatively, *decision tree learning* such as *Classification and Regression Trees* (CART) and *Random Forest* algorithms assorb the patterns that it has learned by encoding as binary rules that split a sample into finer, more homogeneous partitions. Each algorithm has its strengths and weaknesses rooted in how it deals with and assimilates information.

You will no doubt have noticed that the algorithms mentioned sound quite exotic when compared with the plain vanilla regressions in Chapters 8 and 9. There are hundreds of machine learning algorithms that are commonplace in the modern data science workbench, many of which are well-suited for both classification and regression problems. In this chapter, we explore a number of these methods, illustrating their basic properties and their potential role in helping public and social missions.

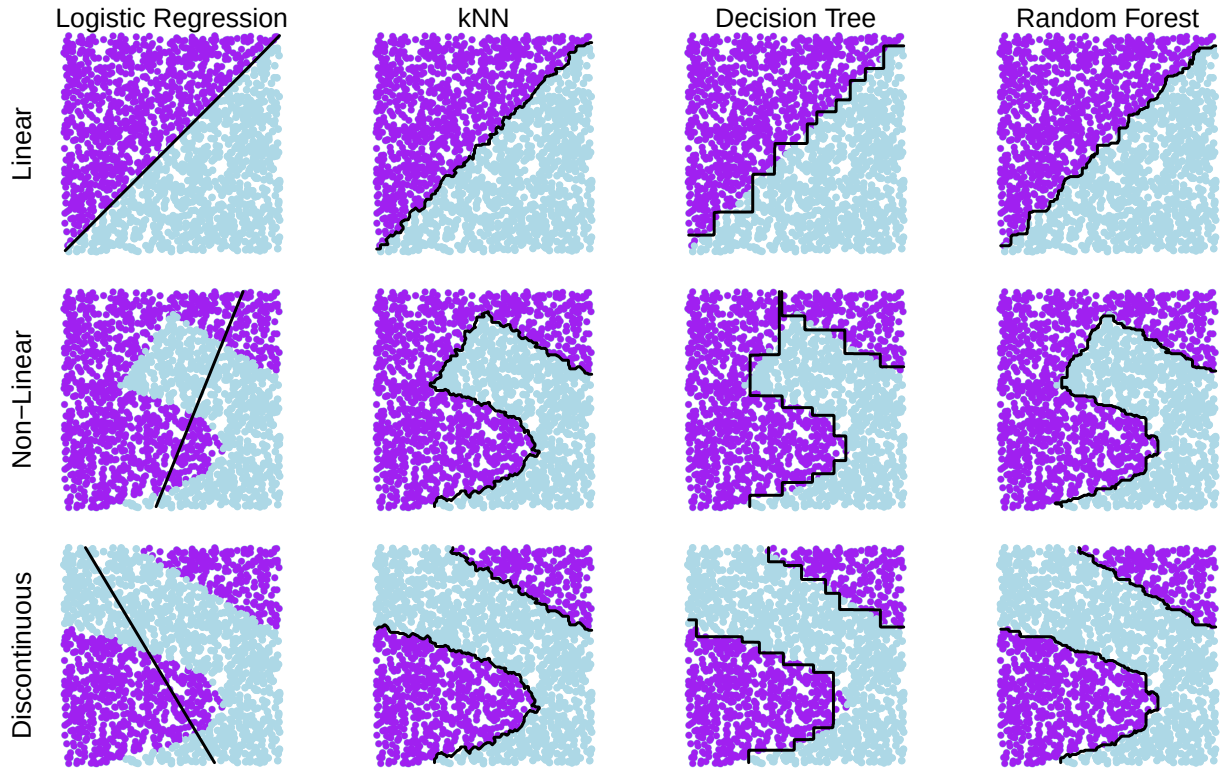


Figure 1.1: Linear, Non-Linear and Discontinuous Classification Problems.

1.2 K-Nearest Neighbors (KNN)

K-nearest neighbors (KNN) is a non-parametric algorithm built on a simple idea: *observations that are closer together are likely to be similar*. This non-parametric technique does not learn coefficients like in the case of regression, but rather treats its input variables X like coordinates in order to measure distance between each other. It is instance-based, meaning that the prediction of each y_i is inferred from each point's surrounding neighbors. In many ways, KNN molds to the data. Since it lacks a formal empirical structure, the algorithm can impute missing values in a realistic, organic fashion.

1.2.1 Under the hood

The algorithm is quite simple. For each case y_i:

1. Calculate distance. First, we calculate the distance d to all other records with known outcomes. Distance most commonly takes the form of Euclidean distance, which is appropriate with continuous values. For cases where the underlying data are boolean or binary, Manhattan distance is more appropriate.

$$\text{Euclidean distance} = \sqrt{\sum_{i=1}^{n}(x_i - x_0)^2}$$

$$\text{Manhattan distance} = \sqrt{\sum_{i=1}^{n}|x_i - x_0|}$$

In effect, the collection of input variables X serve as coordinates and help locate neighborhoods of points.

2. Vote!. For the k nearest observations to a given observation, we calculate the proportion of observations in each class j in Y. This yields a conditional probability for each observation i, which is converted into a predicted class through *majority voting* – assign an observation to the class that is most represented in the neighborhood. There are various flavors of the voting calculation that account for distance from a given observation.

Table 1.1: Types of voting kernels

Voting Type	Formula	Interpretation
Rectangular	$Pr(Y=j) = \frac{1}{k}\sum_{i=1}^{k} I(y^i = j)$	Calculate the proportion of j based on k nearest neighbors.
Inverse	$Pr(Y=j) = \sum_{i=1}^{k} w(d)(y^i = j)$ where $w(d) = \frac{1}{d_i \sum_{i=1}^{k}(\frac{1}{d_i})}$	Calculate the weighted proportion of j based on the inverse distance to k nearest neighbors.
Biweight		
Gaussian		

3. Tune k. The KNN technique is sensitive to the value of k and the voting kernel, requiring tuning – or testing different values of k. When $k = 10$ with a rectangular kernel, the conditional probability for y_i reflects the 10-nearest neighbors. When $k = n$, the conditional probability is equivalent to the sample mean.

KNNs are merely a smoothing procedure. They are highly effective for filling missing data, but their simplicity also does not allow them to learn or store patterns they uncover nor do they facilitate inference.

1.2.2 Working with KNNs

Tuning. Like many other algorithms, KNNs require systematic trial and error in order to optimize the *hyperparameters*. We do not know what is the true value of k or the absolute best kernel to use, thus tuning of the hyperparameters is a necessity, typically relying on a grid search. The idea is to develop a ballpark sense of what works, then hone in on the best value of k. One search strategy could test all values from $k = 1$ to $k = \sqrt{n}$ in multiples of one's choosing, keeping track of how each k performs in terms of a loss function (e.g. TPR, FPR, F1-statistic).

To illustrate the tuning process, we have assembled a sample of USDA CropScape landcover data (W. Han (n.d.)) for farmland that grows corn (yellow) and soybeans (green). More often than not, data will having missing values and capture only a fraction of the full picture. Suppose we had only 10% of all land cover data available, but need to see the remaining 90%. KNNs can impute the likely landcover using available data, tuning the value of k. *Exactly how important is the choice of k?* In the imputations below, we compare values of k at 1, 5, 10, and 100. It is apparent that as the value of k increases, the corn fields increasingly creep into areas where soy would be expected. Not only is this loss in accuracy reflected visually, but statistically as well.

Normalization. Treating variables as coordinates implies that they all should have equal importance – no single variable should weigh on the distance calculation more than any other. Therefore, the scale of each variable should be normalized, at least for continuous variables. For example, if an input variable x_1 has a scale from 1 to 10,000 and x_2 ranges from 0.1 to 0.3, a KNN will lean more heavily on the latter variable. Normalization can be as simple as calculating the z-score for each x_k:

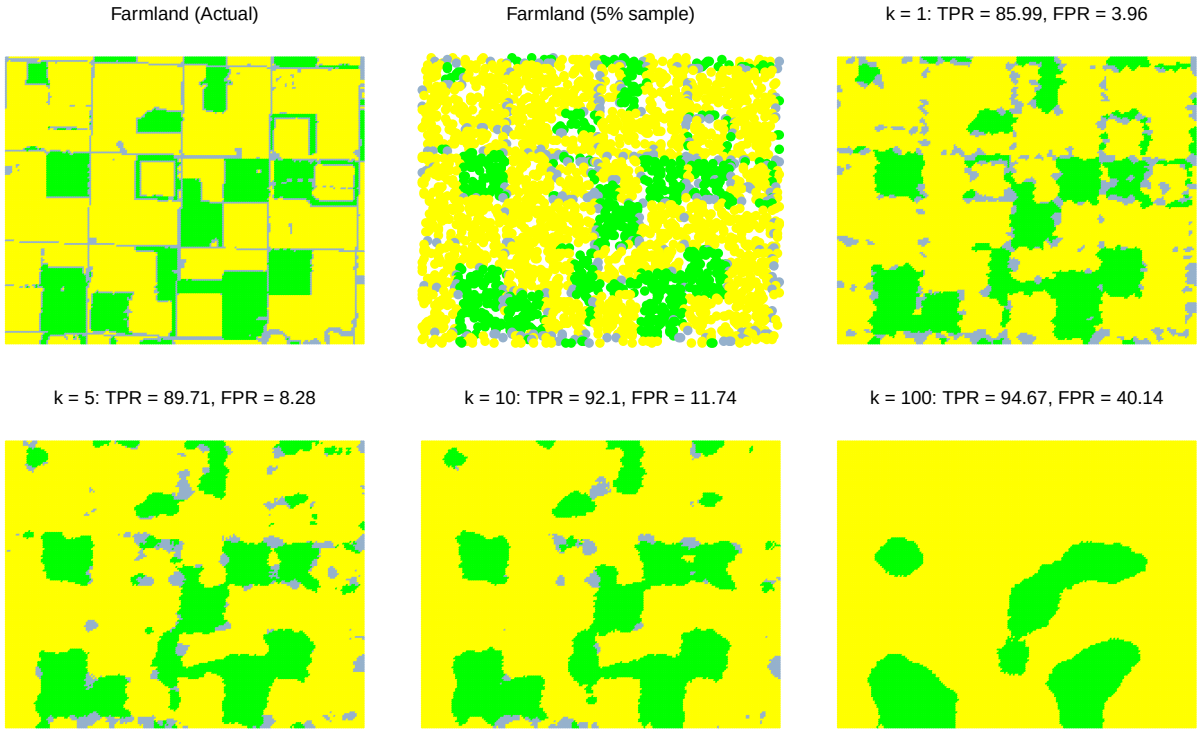


Figure 1.2: Comparison of prediction accuracies for various values of k.

$$scaled = \frac{x_k - \mu_{x_k}}{\sigma_{x_k}}$$

where the transformed variable is mean centered with unit variance.

- *Grids.* Similar to the scale issue, KNNs are particularly effective in data that are distributed on a grid – measurements along a continuous scale at equal incremenets, but may be a poor choice when the data are mixed data formats such as integers and binary.
- *Symmetry.* It's key to remember that neighbors around each point will not likely be uniformly distributed. While kNN does not have any probabilistic assumptions, the position and distance of neighboring points may have a skewing effect.

Usage. KNNs are great in some cases; Not so much in others.

KNNs are commonly associated with imputation of missing values and scenarios where proximity of observations has some bearing on the predictive accuracy. But setting up the KNNs requires some care.

As scale matters, data sets with mixed data types (discrete, continuous) need to be transformed into the same units. Discrete variables can be converted into a dummy variable matrix. Continuous variables can be binned into discrete levels, then converted into a dummy variable matrix as well. This effectively means that all variables are in terms of 0/1 and a Minkowski distance may be more appropriate to relate distances than Euclidean.

KNNs are best used when data sets are relatively smaller with fewer variables as each distance calculation is computationally taxing. Furthermore, as more variables are added, the importance of any one variable is diluted – it may be worth trying another algorithm to sift through the data.

Lastly, KNNs are not interpretable as it is a nonparametric approach. It should be instead be viewed as a processing method to fill in the gaps.

Table 1.2: The good and ugly of KNNs.

Useful Properties	Challenges
Efficient and timely when there are relatively few variables.	Mixed data types require convert all data into dummy matrices
Effective in capturing patterns in cases were proximity matters.	Does not offer an interpretation.
Common choice for imputing missing values.	

1.2.3 DIY: Anticipating the extent of damage from a storm

As hurricanes become more intense and leave a trail of destruction, city governments will need to be able to more efficiently triage requests for help. Let's take the example of Hurricane Sandy and its effect on NYC. One of the main services offered by cities is the management and care of its trees. A downed tree can cause property damage, bodily harm and traffic disruptions. Due to the high wind and lush foliage during Sandy, many trees fell.

In NYC, the Department of Parks and Recreation is responsible for tree removal. When a resident makes a call to the city's services hotline 311, a work order is created and a tree removal team is dispatched. This may be a transactional process: one call for tree removal, one tree is then removed. As it takes time for crews to move and set up, a first-in/first-out queuing process can be inefficient. Imagine if 20 of 100 blocks in a neighborhood were flagged for tree removal. It would make sense to use that call data to identify other blocks that may also have downed trees.

We would expect that downed trees are more likely to occur in *pockets* and proximity is the best indicator of activity. As the city knows where residents call for tree- and non-tree-related issues, we can use the location of the calls to triangulate on likely problem areas as well as anticipate pockets of yet-to-be-reported downed trees, or at least serve that is a reasonable working theory. For this task of predicting based on proximity, k-Nearest Neighbors (KNN) can help. Suppose the location of all calls for non-emergency help from the day of Hurricane Sandy are captured in NYC's 311 system, yet there are still neighborhoods that likely have downed trees but have not reported it. *From what we know, how can we guess the disposition of other parts of the city to have a fuller picture?*

Prepare the data. Some calls for help are associated with downed trees while others may concern non-emergency issues. By this logic, we could assume that a downed tree would be called in if a call were made at all.

Our data set contains $n = 7513$ observations, each of which is a 1000 foot by 1000 foot area. When plotted, the data set captures the outline of NYC.

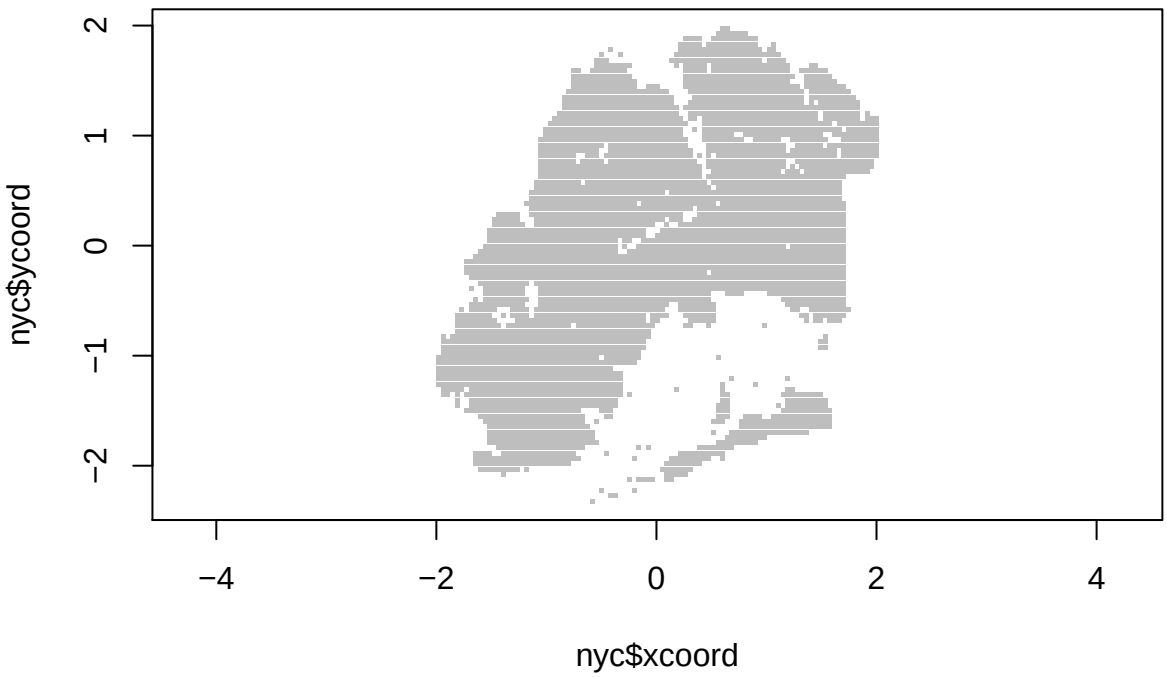
```
#Load data (need persistent link)
  nyc <- read.csv("data/sandy_trees.csv")
```

For simplicity, we will focus on the two largest and geographically connected boroughs, Brooklyn (BK) and Queens (QN). The remaining boroughs of the city are separated by rivers, which may be better represented using separate models. We subset our data using the `boro` variable to focus, scale the geographic coordinates using the `scale` function, and map the resulting subset.

```
#Subset
  nyc <- subset(nyc, boro %in% c("QN", "BK"))

#Standardize input variables
```

```
  nyc$xcoord <- scale(nyc$xcoord)
  nyc$ycoord <- scale(nyc$ycoord)
```



Train. While this is a retrospective analysis, we simulate the process of producing the complete map as if we had partial information. The `nyc` data frame is split into a `train` set, keeping only locations where the target variable `tree.sandy` are available. A quick tabulation shows that the $n = 1550$ of the $n = 1946$ training set observations have a downed tree reported.

```
#Subset training sample
  train <- subset(nyc, !is.na(tree.sandy),
                  select = c("ycoord", "xcoord", "tree.sandy"))

#Split out
  table(train$tree.sandy)
```

```
##
##    0    1
##  396 1550
```

The test set is the entirety of Brooklyn and Queens. The `tree.next7` variable flags any location that had a report of a downed tree over the seven days after the hurricane.

```
  test <- subset(nyc,
                 select = c("ycoord", "xcoord", "tree.next7"))
```

With the data in the right shape, we load the `kknn` library:

```
  library(kknn)
```

The KNN algorithm needs to be calibrated for the best k using the training set, then applied to a test set. To do this, we will use the `kknn` library. The training portion uses the `train.kknn()` function to conduct k-folds cross validation, then the scoring uses `kknn()`. While both functions can be fairly easily written from scratch (and we encourage new analysts to write their own to intimately understand the assumptions), we will plow forth with using the library.

In order to find the optimal value of k, we will execute the `train.kknn()` function, which accepts the following arguments:

`train.kknn(formula, data, kmax, kernel, distance, kcv)`

- `formula` is a formula object (e.g. "`no.coverage ~ .`").
- `data` is a matrix or data frame of training data.
- `kmax` is the maximum number of neighbors to be tested
- `kernel` is a string vector indicating the type of distance weighting (e.g. "rectangular" is unweighted, "biweight" places more weight towards closer observations, "gaussian" imposes a normal distribution on distance, "inv" is inverse distance).
- `distance` is a numerical value indicating the type of Minkowski distance. (e.g. 2 = euclidean, 1 = binary).
- `kcv` is the number of partitions to be used for cross validation.

The flexibility of `train.kknn()` allows for test exhaustively and find the best parameters. Below, we conduct 20-folds cross validation testing between $k = 1$ and $k = 100$ neighbors using two kernels (rectangular and inverse) that impact the voting step. This simple command does much of the hard work by running the KNN algorithm 2000 times (20 cross-validation models for each k and *kernel* combination), then surfaces the best parameters. We store the results in `fit.cv`.

```
#Set seed to ensure cross validation is replicable
  set.seed(100)

#Run with 20-folds cross validation
  fit.cv <- train.kknn(tree.sandy ~ ycoord + xcoord ,
                       data = train,
                       kcv = 20,
                       distance = 1, kmax = 100,
                       kernel = c("rectangular", "inv"))
```

Within `fit.cv` is a `best.parameters` element that KNNs perform the best when $k = $ 59 using an inverse distance kernel.

```
   plot(fit.cv)
```

With the KNN algorithm tuned, we can now proceed to scoring the test set using the `kknn()` function. The function syntax is as follows:

`kknn(formula, train, test, k, kernel, distance)`

- `formula` is a formula object (e.g. "`no.coverage ~ .`").
- `train` is a matrix or data frame of training data.
- `test` is a matrix or data frame of test data.
- `k` is the number of neighbors.
- `kernel` is the type of weighting of distance (e.g. "rectangular" is unweighted, "biweight" places more weight towards closer observations).

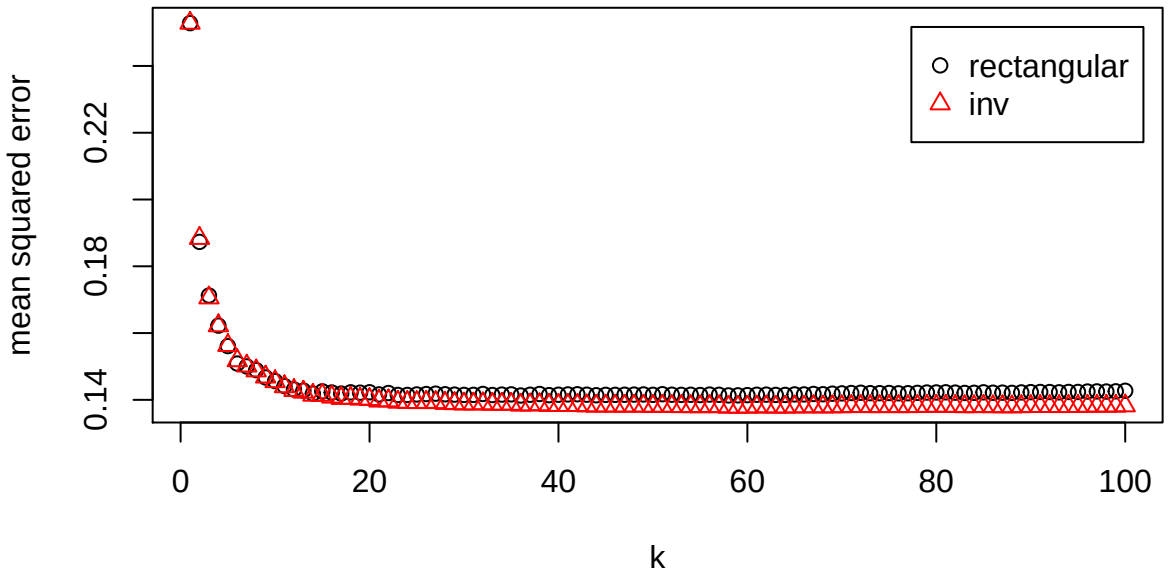


Figure 1.3: 20-fold cross validated errors for k = 1 to k = 100

- `distance` is a numerical value indicating the type of Minkowski distance. (e.g. 1 = binary, 2 = euclidean,).

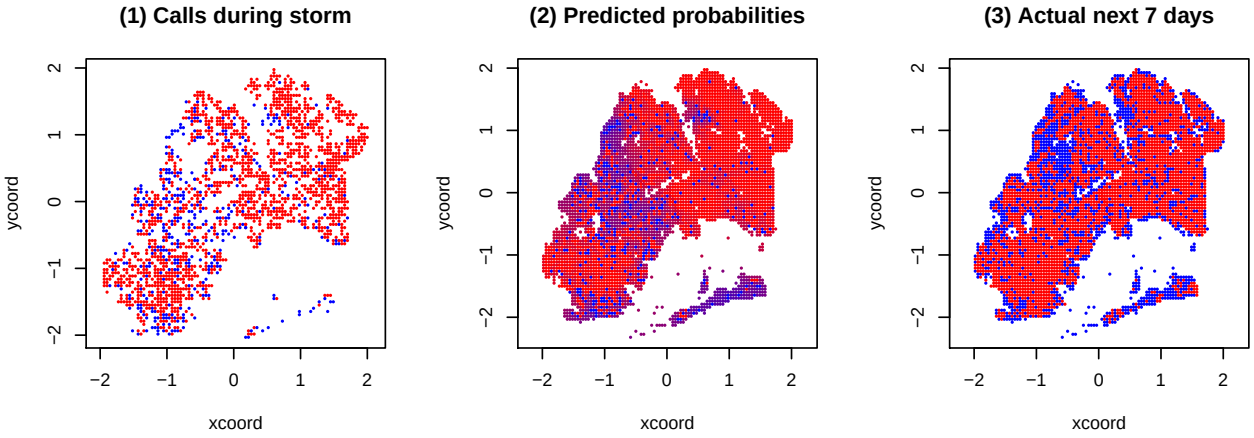
Notice that in the following code block, we train the KNN and apply it to the test sample all in one step as the KNN itself does not learn patterns, but just applies a simple calculation following a pre-specified routine. This is a marked difference compared with other algorithms covered in this chapter.

```
#Retrieve best parameters
   best <- fit.cv$best.parameters

#Apply tune KNN parameters
   fit <- kknn(tree.sandy ~ ycoord + xcoord,
               train = train,
               test = test,
               k = best$k,
               kernel = best$kernel)

#Produce
    test$prob <- fit$fitted.values
    test$tree.next7[is.na(test$tree.next7)] <-0
```

Evaluate. With all the right pieces computed, we can examine how closely the predictions based on tree downing patterns on the day of Hurricane Sandy compare with where trees were reported to have fallen over the 7 days that followed. During the storm, approximately 43% percent of the focus area made a call, of which 80% reported a downed tree. This appears as a cloud of points capturing the gist of the downed tree pattern.



Using the predicted probabilities for the test sample, we calculate the TPR and FPR using both a naive cutoff threshold ($p = 0.5$), finding a high TPR but a FPR of almost similar magnitude. Using such prediction would not provide any insight to field crews.

```
#Calculate FPR and TPR
  tab <- table(test$prob >= 0.5, test$tree.next7)
  tpr <- tab[2,2]/sum(test$tree.next7)
  fpr <- tab[2,1]/sum(test$tree.next7 == 0)
  print(paste0("TPR = ", round(tpr,3), ", FPR = ", round(fpr,3)))
```

```
## [1] "TPR = 0.881, FPR = 0.777"
```

However, a more informed cutoff based on the first day's probability of a downed tree (p = 0.8) yields slightly more balanced results – sacrifiing some true positives for far fewer false positives.

```
tab <- table(test$prob >= 0.8, test$tree.next7)
tpr <- tab[2,2]/sum(test$tree.next7)
fpr <- tab[2,1]/sum(test$tree.next7 == 0)
print(paste0("TPR = ", tpr, ", FPR = ", fpr))
```

```
## [1] "TPR = 0.71188673032598, FPR = 0.390277777777778"
```

The test model accuracy can also be calculated by taking the Area Under the Curve (AUC) of the Receiving-Operating Characteristic. The ROC calculates the TPR and FPR at many thresholds, that produces a curve that indicates the general robustness of a model. The AUC is literally the area under that curve, which is a measure between 0.5 and 1 where the former indicates no predictive power and 1.0 indicates a perfect model.

In order to visualize the ROC, we will rely on the `plotROC` library, which is an extension of `ggplot2`. We will create a new data frame `input` that is comprised of the labels for the test set `ytest` and the predicted probabilities `test.prob`.

```
#Load libraries
  library(ggplot2)
  library(plotROC)

#Set up test data frame
  input <- data.frame(ytest = test$tree.next7,
                      prob = test$prob)
```

We then will first create a ggplot object named `base` that will contain the labels (`d =`) and probabilities (`m =`), then create the ROC plot using `geom_roc()` and `style_roc()`. A ROC curve for a well-performing

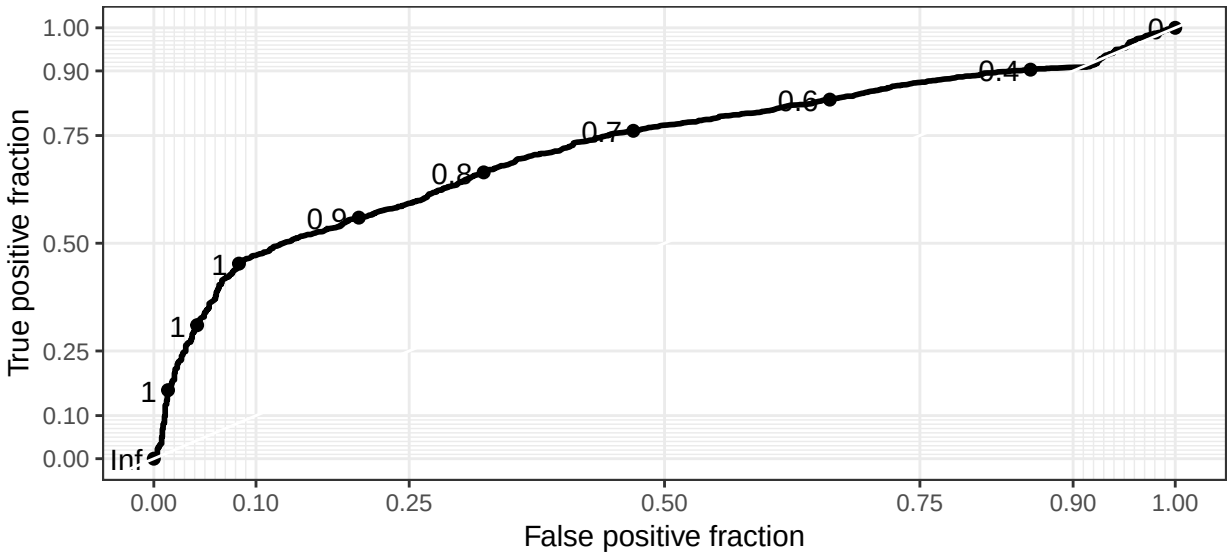


Figure 1.4: ROC curve out of sample

model should sit well-above the the 45 degree diagonal line, which is the reference for an AUC of 0.5 (the minimum expected for a positive predictor). However, as the curve is below the 45 degree line, we may have a seriously deficient model.

```
#Base object
  roc <- ggplot(input, aes(d = ytest, m = prob)) +
         geom_roc() + style_roc()

#Show result
  roc
```

As estimated using `calc_auc()`, the out-of-sample AUC is 0.721, which is not a bad start. While we are able to fill impute the status of downed trees in other parts of the city, it is helpful to remember that the output of the KNN needs to match the intended use. If a limited number of field crews are deployed, then it may more sense to use the probabilities to prioritize neighborhoods. Otherwise, if additional resources could be hired, then knowing the total number of likely affected areas could inform how much to budget for the downed trees effort.

```
  calc_auc(roc)$AUC
```

```
## [1] 0.7205748
```

Despite the promising result, we should be cognizant that KNNs generally are not the algorithm of choice of modelers unless there is relatively little data. We should thus ask: *Is there a better classifier?*

1.2.4 Practice Exercises

The US Census Bureau's American Community Survey provides an in-depth view of life in America. One of the many features that are captured in the survey is healthcare coverage. Apply the above methods to predict healthcare coverage in the US State of Georgia in the year 2009.

1. Randomly split the sample into a 50% training and 50% test set.
2. Predict healthcare `coverage` using continuous variables such as age (`age`) and `wage`.
3. Calculate the performance on the test sample.

1.3 Decision Tree Learning

Mobile technologies have lowered the bar to using lightweight sensors that measure the physical world and have opened new applications of data in daily life. From a smart phone's accelerometer, it's possible to track distinct patterns in one's activity based on the fluctuations in acceleration ($\frac{m}{s^2}$). In fact, many of these technologies have become commonly available, enabling physical fitness activity monitoring to characterizing transportation quality. Below is a set of exercise measurements from an smartphone accelerometer that lasted approximately 6.5 minutes and graphed at a frequency of 5 hertz (five readings per second).

Can you visually identify distinct patterns? What makes those patterns distinct?

It becomes immediately apparent that the methods covered thus far are not suitable for the task at hand. If we manually extract samples from these periods, we can quantify the patterns in terms of their central tendencies. Idle periods have near zero acceleration, walking periods have acceleration around 0.2 with tight dispersion, running periods hover around 0.6 +/- 0.2, and descending stairs vary widely. Using simply the level of acceleration may not accurate as at least two types of motion have overlapping distributions.

Decision tree learning can help bring clarity. Trees are designed to look at inputs and partition the sample into smaller more homogeneous cells with respect to the target. This recursive partitioning allows a tree to resemble an inverted tree: moving away from the base of the tree, the tree trunk splits into two or more large branches, which then in turn split into even smaller branches, eventually reaching even small twigs with leaves.

Decision trees use recursive partitioning to learn patterns, doing so using central concepts of *information theory*. There are a number of decision tree algorithms that were invented largely in the 1980s and 1990s, including the ID3 algorithm, C4.5 algorithm, and Classification And Regression Trees for Machine Learning (CART). All these algorithms follow the same framework that includes the following elements: (1) nodes and edges, (2) attribute tests, and (3) termination criteria.

1.3.1 Under the hood

Anatomy of a decision tree. The tree is comprised of nodes and edges. Nodes (circles) contain records. Edges (lines) show dependency between nodes and is the result of an *attribute test* – or a process that finds the optimal criterion to subset records into more homogeneous groups of the target variable. The node at the top of the tree is known as the *root* and represents the full population. Each time a node is split, the result is two nodes – each of which is referred to as a *child node*. A node without any child nodes is known as a *leaf*. The node is labeled using majority voting based on whichever class is most represented. The goal is to grow a tree from the root node into as many smaller child nodes that contain more of one class than another.

Decision trees split nodes based on finding thresholds along the input variables. There can be seemingly infinite number of potential variable-threshold combinations – which is best? Drawing from *information theory*, we can apply an *information gain* formula to evaluate all candidate splits and find one that provides the most information. This optimal split yields to more homogeneous child nodes, which in turn can be split even further. The search for the best threshold is known as an *attribute test*.

As we can see in the example decision tree for health care insurance, each node is connected to at least one other node. Starting at the root node, we can see that overall, the population is labeled "no coverage" based on the decimal percentage 0.5. The 100% indicates the proportion of the sample that is contained at the node. Below is `age >= 64`, which is the most informative attribute test that is used to split. To the left, the edge leads to another node at the bottom left corner of the diagram, which contains people who are age 64 or older. While the leaf node only contains 12% of the entire sample, it is almost exclusively people who have health care coverage. To the right, the remaining 88% of the sample, which is further split by wage and other variables. Each leaf node is defined as the intersection of multiple binary criteria, giving way to profiles of users that can be easily segmented.

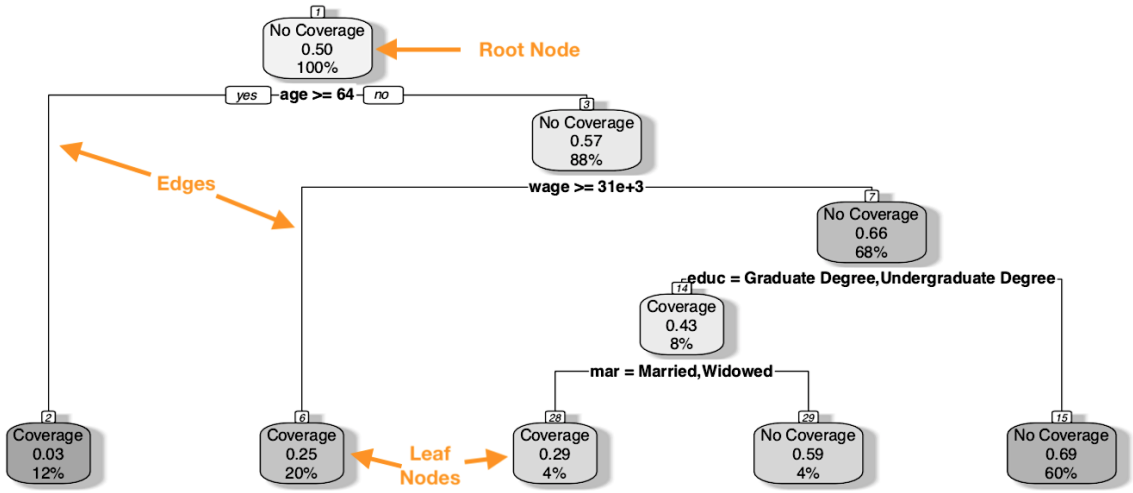


Figure 1.5: Anatomy of a Decision Tree.

Growing trees. There are a number of decision tree algorithms that were invented largely in the 1980s and 1990s, including the ID3 algorithm, C4.5 algorithm, and Classification And Regression Trees for Machine Learning (CART). The process is fairly clear cut and iterative:

1. **Base Cases**. The process starts with checking for "base cases" at the root node, the idea being that it might not be worth exerting effort to grow the tree if the data do not support it. The algorithm will first check to see if (a) all values of the target are of one class, and (b) none of the input variables offer any useful information. There are other base cases to consider depending on the algorithm, but any true base case will result in stopping the algorithm and returning only the root node.

2. **Recursive Partitioning**. If none of the base cases are true, the algorithm proceeds to attribute testing using either *Information Gain* or *Gini Impurity* as will be covered in the following section. At the root node, if there are 10 variables with each 30 possible thresholds, attribute tests are applied 300 times choosing the candidate threshold that yields the most homogeneous child nodes. Upon splitting, attribute tests are applied to each child node, making this a recursive partitioning procedure.

3. **Stopping Criteria versus Pruning**. At some point, the algorithm needs to stop. The question is *when*? One way is to grow the tree until some *stopping criteria* are met, such as if a leaf has fewer records than a pre-specific threshold, the purity or information gain falls below a pre-specified level, or if the tree has grown to n-number of levels (e.g. number of rows of splits). While stopping criteria are useful, the results in some studies indicate their performance cap the tree from reaching its full predictive potential.[1] The alternative approach involves growing a tree to its fullest, then comparing the prediction performance given tree complexity (e.g. number of nodes in the tree) using cross-validation. In the example graph below, model accuracy degrades beyond a certain number of nodes. Thus, optimal number of nodes is defined as when cross-validation samples (e.g. train/test, k-folds) reaches a minimum across samples. Upon finding the optimal number of nodes, the tree is *pruned* to only that number of nodes.

Attribute Tests. Information gain is a form of *entropy* that measures the consistency of information. Based on these distinct states of activity, entropy is defined as:

$$\text{Entropy} = \sum_{i=1}^{k} -p_i log_2(p_i)$$

[1]

where i is an index of states, p is the proportion of observations that are in state i, and $log_2(p_i)$ is the Base 2 logarithm of the proportion for state i. Information Gain (IG) is variant of entropy, which is the entropy of the root node *less* the average entropies of the child nodes.

$$\text{IG} = \text{Entropy}_{\text{root}} - \text{Avg Child Entropy}$$

How does this work in practice? Starting from the root node, we need to calculate the root entropy, where the classes are based on the classes of the target `usership`.

$$\begin{aligned}\text{Entropy}_{\text{usership}} &= (-p_{user} log_2(p_{\text{user}})) - (-p_{\text{non-user}} log_2(p_{\text{non-user}})) \\ &= (-\tfrac{6}{12} log_2(\tfrac{6}{12})) + (-\tfrac{6}{12} log_2(\tfrac{6}{12})) \\ &= 1.0\end{aligned}$$

Then, the attribute test is applied to the root node by calculating the weighted entropy for each proposed child node. Using the `income` feature, the calculation is as follows:

- Split the root node into two child nodes using the `income` class. This yields the following subsamples as shown in the table below:

	$<$ \$20k	$>$ \$20k
No	0	6
Yes	5	1
Total	5	7

- For each child node (the columns in the table), calculate entropy:

$$\begin{aligned}\text{Entropy}_{\text{income} < \text{20k}} &= (-p_{user} log_2(p_{\text{user}})) - (-p_{\text{non-user}} log_2(p_{\text{non-user}})) \\ &= -\tfrac{5}{5} log_2(\tfrac{5}{5}) = 0 \\ \text{Entropy}_{\text{income} > \text{20k}} &= (-p_{user} log_2(p_{\text{user}})) - (-p_{\text{non-user}} log_2(p_{\text{non-user}})) \\ &= -\tfrac{6}{7} log_2(\tfrac{6}{7}) + -\tfrac{1}{7} log_2(\tfrac{1}{7}) = 0.5916728\end{aligned}$$

- Calculate the weighted average entropy of children:

$$\text{Entropy}_{\text{income split}} = \tfrac{5}{12}(0) + \tfrac{7}{12}(0.5916728) = 0.3451425$$

- Then calculate the information gain:

$$\begin{aligned}\text{IG}_{\text{income}} &= \text{Entropy}_{\text{root}} - \text{Entropy}_{\text{income split}} \\ &= 1 - 0.3451425 = 0.6548575\end{aligned}$$

- We then can perform the same calculation on all other features (e.g. employment, part of town) and compare results. The goal is to *maximize* the IG statistic at each decision point. In this case, we see that income is the best attribute to use for splitting. This split is easily interpretable: "The majority of users of health services can be predicted to earn less than \$20,000."

Measure	IG
Employment	0.00
Income	0.6548575
Area of Town	0.027119

Gini Impurity is closely related to the entropy with a slight modification.

$$\text{Gini Impurity} = \sum_{i=1}^{k} p_i(1-p_i) = 1 - \sum_{i=1}^{k} p_i^2$$

Using Gini Impurity as an attribute test is also similar to Information Gain.

$$\text{Gini Gain} = \text{Gini}_{\text{root}} - \text{Weighted Gini}_{\text{child}}$$
$$\Delta i(s,t) = i(t) - p_L i(t_L) - p_R i(t_R)$$

1.3.2 Tips of the trade

Like any technique, decision trees have strengths and weaknesses. Unlike logistic regression and KNN, decision trees can conduct automated variable selection on any type of data type. In addition, the recursive partitioning produce a tangible definition for each subpopulation represented by a node. The splitting mechanism make it possible to capture interactions and non-linearities that are otherwise not easily accounted for in the previous methods. The implications are that two or more input variables can be blended together to find cells of activities that are otherwise overlooked.

There are detractors, however. Trees can be grown so deeply that there are too many subpopulations to articulate. If left unpruned, terminal leafs may give a false impression of accuracy and precision – the small samples may give a false impression. Nontheless, decision tree learning is an important contribution to classification problems and form the basis of many other algorithms.

Table 1.5: The good and ugly of decision trees.

Useful Properties	Challenges
Rules (e.g. all the criteria that form the path from root to leaf) can be directly interpreted.	Data sets with large number of features will have overly complex trees that, if left unpruned, may be too voluminous to interpret.
Method is well-suited to capture interactions and non-linearities in data.	Trees tend to overfitted at the terminal leafs when samples are too small.
Technique can accept both continuous and continuous variables without prior transformation.	Feature selection is conducted automatically.

1.3.3 DIY: Predicting monetary and non-monetary relief

> Navient has been unresponsive after I've asked to speak with several managers. I have called them consistently since summertime as my automatic payments were not being taken out. They say it came back as NSF, but my bank says it was never billed. Then Navient admitted to having I.T. issues. Late fees, interest, you name it. After calling to resolve many times, they offered me payment options and promised to repair my credit damage of their reporting me. After making each payment, they would change the terms and tell me I had to pay additional money or pay this or that, and then they would rescind the negative info. I finally scraped up the money and paid what it said I was past due on after their lies - and the online account still shows I owe money as of {xx/xx/xxxx} and its {xx/xx/xxxx} - so my payment made on {xx/xx/xxxx} obviously didn't post although it was taken from my bank account. I called again today and requested that a manager call me back - nothing yet. Supposedly they record all calls - well, someone should listen to all the lies they've been telling me over the months and changing the agreements. It is unethical and immoral. They are ruining students lives! Check the recordings and the call logs - I'm the one who calls them! And if they ever seldom call me, they never leave a voicemail but

> the recordings will prove they lie and say they did leave a voicemails, and I dispute that and tell them they are lying directly. listen to the recordings!

This is a complaint written by a real consumer of a non-federal student loan and filed with the Consumer Financial Protection Bureau (CFPB). Designed for the purpose of providing consumers help in navigating difficulties with financial products, CFPB collects [].

For transparency, CFPB publishes complaint narratives as an open, anonymized database that indicates the disposition of cases and their details. Looking at the text above, certain words and phrases signal nature of them problem and the word choice also signals the sentiment of the users. Those details, in turn, may explain whether companies provide the consumer any relief, whether monetary or otherwise.

Imagine a scenario in which we would like to anticipate the outcome of a case or the label of a document before its available, but the only covariates are embedded in the text. A large team of people could read through and assign tags to each piece of text to generate usable covariates, but this is a long arduous task requiring significant manpower. Alternatively, what if we forced the unstructured text into a structure similar to data sets we have encountered before? Each narrative can been *tokenized*. First, text is standardized through stemming word endings (e.g. tell, tells, and telling all become "tell"), then are processed into *n-grams* of individual words and short word sequences. For example, "*the online account still shows I owe money*" contains eight unigrams (e.g. the, online, account, still, shows, I, owe, money), seven bigrams (e.g. the online, online account, account still, still shows, shows I, I owe, owe money), and six trigrams (e.g. the online account, online account still, account still shows, still shows I, shows I owe, I owe money). In total, the sentence yields a *bag of words* of 21 variables. Of course, some of these words are filler (e.g. "the", "I") and can be treated as *stop words* or words that can be removed as they do not likely contain signal. Combinations of these n-grams are the key to understanding what is associated with monetary relief – it is a game of interactions that is well-suited for CART algorithm.

In this DIY, we explore how CART the power of a non-parametric approach can learn the intracies in text. Covering a 49-month period from March 2015 to March 2019, we have pre-processed CFPB data into a training set (n = 9519) and test set of the remaining years (n = 49547). Note that the training set is smaller than the test for ease of computation as text data sets tend to be highly dimensional. In fact, the pre-processed training set had 469,046 unique n-grams, but was reduced to the one-percent of tokens ($k = 4657$) with three or more character and appear ten or more times in 2015. For more on the mechanics of working with unstructured textual data, refer to the advanced topics chapter.

```
#Load CFPB data
  load("data/cfpb_dtm.Rda")
```

Training. Our primary target is the `target.series` variable that includes labels for *Closed with non-monetary relief* and *Closed with monetary relief*. There is a slight case of class imbalance, but so severe to require re-balancing.

```
#Quick summary
  table(train$target.series)
```

```
##
##     Monetary Non-monetary
##         4894         4625
```

A cursory view of the frequency of words gives some indication of the structure of the narratives. The most frequent words help set the stage. CART will likely use less frequent words to modulate its predictions, relying on finer, thematic details to inform its predictions. Some words

We make use of CART using the `rpart` library.

Table 1.6: Sample words frequencies.

High		Medium		Low	
Variable	Frequency	Variable	Frequency	Variable	Frequency
account	18843	capit.system	18	frivol	2
credit	12972	capitol	18	furiou	2
call	9597	contest	18	gather	2
payment	8801	custom.repres	18	greatli	2
bank	8476	dealer.servic	18	groceri.store	2
card	7914	dear	18	guilti	2
report	7395	essenti	18	hate	2
charg	6878	fraud.investig	18	heavi	2
receiv	6103	ga.station	18	held.respons	2
told	4924	gc.servic	18	highli	2

```
pacman::p_load(rpart)
```

The main function within the library comes with flexible capabilities to induct decision trees:

`rpart(formula, method, data, cp, minbucket, minsplit)`

where:

- `formula` is a formula object. This can take on a number of forms such as a symbolic description (e.g. $y = f(x_1, x_2, ...)$ is represented as "`y ~ x1 + x2`).
- `method` indicates the type of tree, which are commonly either a classification tree "class" or regression tree "anova". Split criteria can also be custom written.
- `data` is the data set in data frame format.
- `cp` is a numeric indicates the complexity of the tree. $cp = 1$ is a tree without branches, whereas $cp = 0$ is the fully grown, unpruned tree. If cp is not specified, `rpart()` defaults to a value of 0.01.
- `minbucket` is a stopping criteria that specifies the minimum number of observations in any terminal leaf.
- `minsplit` is a stopping criteria that specifies the number of observation in a node to qualify for an attribute test.

As a first pass, we'll run `rpart()` setting `cp = 0`, meaning that the tree will be fully grown without any stopping criteria applied. It may take the CART algorithm a few minutes to learn the patterns in the words.

```
fit <- rpart(target.series ~ .,
             method = "class",
             data = train[, -c(1:5)],
             cp = 0)
```

The `fit` object captures all of the inner workings of the decision tree. For example, just plotting the fit object will show the full depth of the tree. More importantly is the cross validation results collected at each level of additional complexity. Using the `printcp()` function, we can extract the *CP table*, which contains various accuracy measures associated with each value of the tree complexity value `cp`, including:

- the number of splits `nsplit`,
- the prediction error in the training data `rel error`,
- the cross-validation error `xerror`, and
- the standard error `xstd`.

Table 1.7: First five levels of a CP table showing cross validated error by model compexity

CP	nsplit	rel error	xerror	xstd
0.277	0	1.000	1.000	0.011
0.042	1	0.723	0.741	0.010
0.030	4	0.576	0.603	0.010
0.022	5	0.546	0.547	0.009
0.013	6	0.525	0.545	0.009

```
  printcp(fit)
```

Tuning. *How do we find the optimal tree depth?* First, find the lowest cross-validation `xerror`, then find the tree that has the lowest number of splits that is still within one standard deviation `xstd` of the best tree[2]. The idea behinds this rule of thumb takes advantage of uncertainty: the true value lies somewhere within a confidence interval, thus any value within a tight confidence interval of the best value is approximately the same. In this first model, the best tree has nsplit = 32 and xerror = 0.45427027027027. By applying the rule, the upper bound of acceptable error is xerror = 0.45427 + 0.008749 = 0.463019081383439. As it turns out, the tree with nsplit = 27 is within one standard deviation and is thus the best model.

In other words, the following function can extract the optimal `cp` value.

```
bestCP <- function(fit_obj){
  ## Returns best CP val within 1 SD of lowest xerror
  #
  ## Args:
  ##   fit_obj: decision tree object
  #

  #Pull cross-validated error
    xerror <- fit$cptable[, 4]

  #Find lowest error and associated xstd
    best_error <- min(xerror)
    best_sd <- fit$cptable[, 5][which(xerror == best_error)]

  #Pull CP closest to lower bound
    lower_bound <- best_error + best_sd
    opt_select <- fit$cptable[,1][which(xerror <= lower_bound)][1]

   return(opt_select)
}
```

Now, we can prune the tree using the optimal `cp` value, then score both the test set. As a comparison point, we will also apply the unpruned model as well.

```
#Get best CP
  best_value <- bestCP(fit)

#Prune tree
```

[2](???)

```
  fit.opt <- prune.rpart(fit, cp = best_value)

#Score, returning probabilities
  pred.full <- predict(fit, test, type = 'class')
  pred.opt <- predict(fit.opt, test, type = 'class')
```

What works. One of the fascinating aspect of CART is its interpretability. Each terminal node is a set of binary criteria, making it possible to articulate under what conditions can the target occur. This is a reasonable mode of interpretable when trees are relatively simple. Alternatively, CARTs can be reviewed through variable importance that builds upon the *impurity* measures used to construct the trees.

A split in a tree is given as

total impurity less remaining impurity

$$\Delta i(s,t) = i(t) - p_L i(t_L) - p_R i(t_R)$$

$p_L = \frac{N_{t_L}}{N_t}$ $p_R = \frac{N_{t_R}}{N_t}$

gini impurity

$$i(s,t) = 1 - \sum_{i=1}^{J} p_i^2$$

Variable X_m $v(s_t)$ is the variable used in split s_t

Mean Decrease Impurity or Gini Importance

$$Imp(X_m) = \frac{1}{N_T} \sum_{T} \sum_{t \in T: v(s_t) = X_m} p(t) \Delta i(s_t, t)$$

Where *Variable Importance* for variable k is the sum of *Goodness of Fit* (e.g. Gini Gain or Information Gain) at a given split involving variable k. In other words, a variable's importance is the sum of all the contributions variable k makes towards predicting the target. Below, we can see that the measure can be extracted from the `fit.opt` object. As may be expected, `accel` is not the main contributor to predictions, but rather measures of the maximum, mean and variability of acceleration. This also implies that the model could be further tuned by trying different windows for producing the engineered variables – perhaps shorter or longer windows could be even more important.

```
  fit.opt$variable.importance
```

When applied to the function to the predictions (`pred.opt` and `pred.full`), we find that the mean F1-statistics reached `meanF1(test$activity, pred.opt)` and `meanF1(test$activity, pred.full)` – not bad for a first cut, but certainly can benefit from extra attention.

1.4 Random Forests

How do we know anything for sure? Virtually every aspect of life has some uncertainty tied in. When a hurricane approaches the US Eastern Seaboard, forecasters often map the *cone of uncertainty* that provides the possible range of motion of a storm based on the results of many forecasted simulations. In presidential

Table 1.8: Words with high, medium and low importance for predicting monetary relief.

High		Medium		Low	
Variable	Impurity	Variable	Impurity	Variable	Impurity
report	585.111	close.cost	1.986	NA	NA
charg	455.559	close.disclosur	1.986	NA	NA
credit.report	268.365	creditor	1.882	NA	NA
bank	208.821	violat	1.882	NA	NA
card	104.090	alleg	1.838	NA	NA
close	69.498	citigold.check	1.832	NA	NA
experian	55.761	manag	1.758	NA	NA
check	51.517	direct.deposit	1.686	NA	NA
monei	45.922	aadvantag.mile	1.684	NA	NA
late.fee	45.250	citigold.account	1.684	NA	NA

elections, often times the most polling results are ones that ensemble or average the results of many other similarly conducted polls. The reliance on predictions from a group of models with the same aims may well improve prediction accuracy. In statistical learning, average the results of multiple models is known as *ensemble learning* or *ensembling* for short.

Single models may imposes biases on data and may be well-suited in specific situations. Ensemble methods combine the results of many models to obtain more stable results. For example, the curve in graph #1 can be approximated using a decision tree algorithm. The result of a single tree only loosely fits the curve in a jagged fashion (#2). That one tree may impose biases on the data, perhaps through how the tree is pruned or the assumption that the jagged approximation is appropriate, which may then translate into greater variance in predictions. One could imagine that the structure of that one tree may have happened by chance, and under different situations, the fit could be better.

Bootstrapping can help. Recall from elementary statistics that bootstrapping is defined as any statistical process that involves sampling records with replacement. By bootstrapping a sample, we treat a sample like a population, we can expose and characterize the qualities of an estimator under various scenarios already available in the data, which in turn produces an empirical probability distribution for predictions using the estimator. We can bootstrap the decision tree by (1) sampling the data with replacement up to the full size of the sample, then (2) run the decision tree. The result of repeating the process 50 times is (graph #3) produces a result that appears to be more organic and more accurate. This process of *bootstrapping* and *aggregating* the results is referred to as *bagging*.

Applying bagging to decision trees may not necessarily be enough to develop a well-balance prediction. In the social sciences and public policy, it is generally assumed that a model's specification is a choice left to the analyst; However, it may also be a source of methodological bias.

Random forests can help. The technique is an extension of decision trees using a modified form of bootstrapping and ensemble methods to mitigate overfitting and bias issues.[3] Not only are individual records bootstrapped, but input features are bootstrapped such that if K variables are in the training set, then k variables are randomly selected to be considered in a model such that $k < K$. Each bootstrap sample is exhaustively grown using decision tree learning and is left as an unpruned tree. The resulting predictions of hundreds of trees are ensembled. The logic is described below.

Pseudo-code

```
Let S = training sample, K = number of input features
```

[3]Breiman (2001)

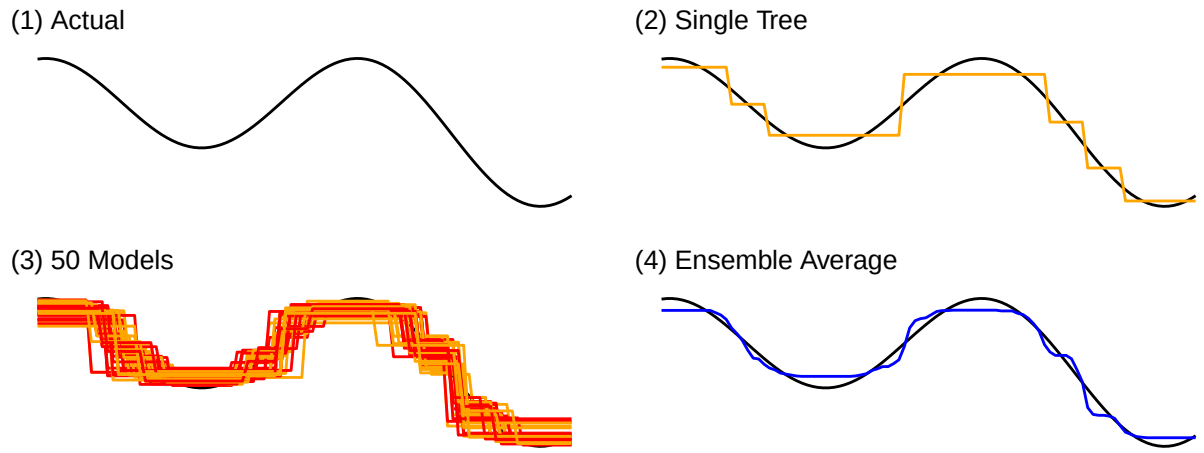


Figure 1.6: Comparison of results of applying a single model to fit a curve versus an ensemble of models.

```
  1. Randomly sample S cases with replacement from the original data.
  2. Given K features, select k features at random where k < K.
  3. With a sample of s and k features, grow the tree to its fullest complexity.
  4. Predict the outcome for all records.
  5. Out-Of-Bag (OOB). Set aside the predictions for records not in the s cases.
Repeat steps 1 through 5 for a large number of times saving the result after each tree.
Vote and average the results of the tree to obtain predictions.
Calculate OOB error using the stored OOB predictions.
```

The *Out-Of-Bag* (OOB) sample is a natural artifact of bootstrapping: approximately one-third of observations are naturally left un-selected, which can be used as the basis of calculating each tree's error and the overall model error. Think of it as a convenient built in test sample.

How about interpretation? Unlike decision trees, it is not a simple task to deduce rules or criteria that describe the target variable. Instead, random forests use *variable importance*, which, like for a decision tree, measures the contribution of a feature to the homogeneity of a classifier. Unlike decision trees, variable importance for a Random Forest is calculated as the mean decrease in the Gini coefficient of a split relative to the Gini coefficient of the root node. Gini coefficients measures homogeneity on a scale of 0 to 1, where 0 is perfect homogeneity and 1 is perfect heterogeneity. The Gini changes are summed for each variable and normalized.

1.4.1 Tuning

Whereas methods like regression have a closed form solution, Random Forest require tuning as optimal models need to be searched for under different conditions. The principal tuning parameters include: Number of features and number of trees.

- *Number of input features.* As k number of parameters need to be selected in each sampling round, the value of k needs to minimize the error on the OOB predictions.
- *Number of trees* influences the stability the Variable Importance metric that is commonly used to infer variable influence in decision tree learning. More trees help to stabilize the Variable Importance estimate. To determine the number of trees, keep adding trees to a sample until the OOB error for a randomly select set of trees is approximately equal to that of the ensemble.

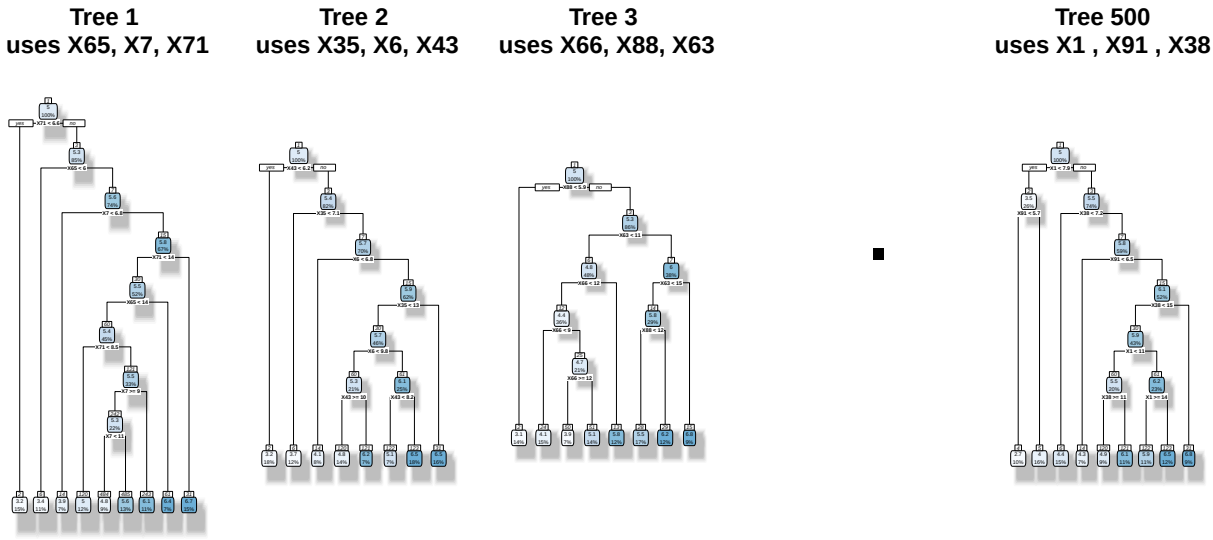


Figure 1.7: Random Forests construct hundreds of trees sampling from both observations and features, then combine the trees into one prediction through voting.

1.4.2 DIY: Revisiting monetary relief

There are a number of R libraries that implement the Random Forest algorithm. The more commonly used version is `randomForest` as it automates most of the procedure, but is less scalable and efficient than its younger sibling `ranger`. As we will revisit the bag-of-words data set in this DIY, the `ranger` library will vastly reduce the time required to train the Random Forest. The `ranger` function expects at least a formula and a data frame,

```
ranger(formula, data, mtry, numtree)
```

where: - `formula` is an expression of the model to be train. The target variable should be in factor format. - `data` is a data frame. - `mtry` (optional) is the number of variables to be randomly sampled per iteration. Default is $\sqrt{k}$ for classification trees. Default set to the square root of the number of variables. - `ntree` (optional) is the number of trees. Default is 500. - `importance` (optional) needs to be specified as "impurity" in order to retrieve variable importance measures. - `num.threads` (optional) is a speed enhancing option that allows the many repetitive steps of a Random Forest to be parallelized across multiple cores or CPUs. By default, `ranger` uses the number of CPUs available.

Using the same formula as the `rpart()` function, we can train a Random Forest with default settings and check the OOB error.

```
#Load randomForest library
  pacman::p_load(ranger)

#Run Random Forest
  fit.rf <- ranger(target.series ~ .,
                   data = train[, -c(1:5)],
                   num.trees = 500,
                   importance = "impurity")
```

```
## Growing trees.. Progress: 23%. Estimated remaining time: 1 minute, 41 seconds.
## Growing trees.. Progress: 43%. Estimated remaining time: 1 minute, 22 seconds.
## Growing trees.. Progress: 51%. Estimated remaining time: 1 minute, 28 seconds.
## Growing trees.. Progress: 70%. Estimated remaining time: 53 seconds.
```

Table 1.9: Sample words frequencies.

High		Medium		Low	
Variable	Frequency	Variable	Frequency	Variable	Frequency
charg	202.843	final.payment	0.162	compani.polici	0.003
report	176.480	revok	0.162	pai.servic	0.003
bank	119.372	stoneg.mortgag	0.162	nt.worri	0.003
card	87.293	fargo.credit	0.162	origin.account	0.003
credit.report	71.066	integr	0.161	inform.request	0.003
debt	58.299	atm.withdraw	0.161	miss.call	0.003
check	49.193	truck	0.161	excess.amount	0.003
monei	43.099	town	0.161	nt.appli	0.003
transact	36.940	circl	0.161	sale.price	0.003
collect	35.603	renov	0.161	receiv.bill	0.003

```
## Growing trees.. Progress: 90%. Estimated remaining time: 18 seconds.
```

Approximately 75.6% of observations in the OOB sample were correctly classified using randomly selected variables in each of the 500 trees.

The `fit.rf` records a number of model outputs such as variable importance calculated as the Mean Decrease Gini. However, the values themselves do not have any meaning outside of a comparison with other Gini measures.

```
  fit.rf$variable.importance
```

By default, the `ranger` library sets the number of trees to equal 500. But what if we would like to find the model that optimizes predictive accuracy? Random Forest algorithms can be tuned by the number of underlying trees in the forest (`num.trees`), the number of variables sub-sampled for any given tree (`mtry`), the minimum node size of terminal nodes (`min.node.size`) among others.

As we know that $n = 500$ trees is more than enough, we will now need to tune the tree for the number of variables. To tune the algorithm, we will use the `tuneRF()` method. The method searches for the optimal number of variables per split by incrementally adding variables. While it's a useful function, it is relatively verbose. In addition to the target and input features, a number of other parameters need to be specified:

```
tuneRF(x, y, ntreeTry,  mtryStart, stepFactor, improve, trace, plot)
```

where: - `x` is a data frame or matrix of input features. - `ntreeTry` is the number of trees used in each iteration of tuning. - `mtryStart` is the number of variables to start. - `stepFactor` is the number of additional variables tested per iteration. - `improve` is the minimum relative improvement in OOB error for the search to go on. - `trace` is a boolean that indicates where to print the search progress. - `plot` is a boolean that indicates whether to plot the search results.

Below, we conduct a search from `mtryStart = 1` with a `stepFactor = 2`. The search result indicates that 2 variables per tree are optimal.

```
library(caret)
data(iris)

grid_params <-  expand.grid(mtry = c(1,4),
                            min.node.size = 1,
                            splitrule = "gini")
```

```
fitControl <- trainControl(method = "CV",
                           number = 5,
                           verboseIter = FALSE)

fit = train(
  x = iris[ , names(iris) != 'Species'],
  y = iris[ , names(iris) == 'Species'],
  method = 'ranger',
  num.trees = 200,
  tuneGrid = grid_params,
  trControl = fitControl
)
```

Normally, we can plug the tuned parameter back into the `randomForest()` method and re-train the algorithm, but it unnecessary in this case as the default model already uses the same parameters. When applied to the test set, we see that the mean F1-statistic is much improved – or a whole 10-percentage point increase.

```
#Predict classes in test
  yhat <- predict(fit.rf, test)
```

This result does not mean that Random Forests will always turn better results, but rather multiple techniques should be tested when tackling prediction problems. Also, remember the policy goal: is the objective to predict or to explain? If a little of both, then it is worth understanding the value of increased accuracy at the cost of interpretability.

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