Notes 6 - Verification Methods

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Math 3190

Section 1

Evaluation Metrics and the Confusion Matrix

Evaluation Metrics

Before we start describing approaches to optimize the way we build algorithms, we first need to define what we mean when we say one approach is better than another.

We use the `caret` package, which has several useful functions for building and assessing machine learning methods.

```
library(tidyverse)
library(caret)
```

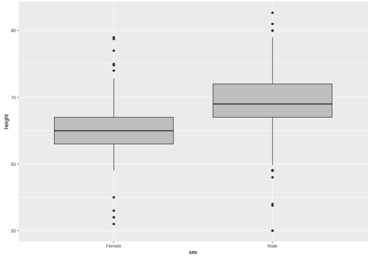
Evaluation Metrics

For a first example, we use the height data in `dslabs`:

```r
library(dslabs)
data(heights)
```

To summarize the data, consider the following boxplot:

```r
ggplot(heights, aes(x = sex, y = height)) +
  geom_boxplot(fill = "gray")
```



Evaluation Metrics

We will start with a simple example: suppose we want to predict sex using height. We start by defining the outcome and predictors.

```
y <- heights$sex
x <- heights$height
```

Evaluation Metrics

In this case, we have only one predictor, height, and `y` is clearly a categorical outcome since observed values are either `Male` or `Female`.

We know that we will not be able to predict Y very accurately based on X because male and female average heights are not that different relative to within group variability. But can we do better than guessing? To answer this question, we need a quantitative definition of better.

Training and Test Sets

Ultimately, a machine learning algorithm is evaluated on how it performs in the real world with completely new datasets. However, we usually have a dataset for which we know the outcomes, as we do with the heights: we know the sex of every student in our dataset. Therefore, to mimic the ultimate evaluation process, we typically split the data into two parts and act as if we don't know the outcome for one of these.

We refer to the group for which we know the outcome, and use to develop the algorithm, as the **training** set. We refer to the group for which we pretend we don't know the outcome as the **test** set.

Training and Test Sets

The caret package includes the function createDataPartition that helps us generates indexes for randomly splitting the data into training and test sets:

```
set.seed(2024)
test_index <- createDataPartition(y, times = 1,
                                  p = 0.5, list = FALSE)
```

The argument times is used to define how many random samples of indexes to return, p is used to define what proportion of the data is represented by the index, and list is used to decide if we want the indexes returned as a list or not.

If times = 1, this is essentially the same as doing

```
set.seed(2024)
test_index <- sample(1:nrow(heights),
                     size = round(nrow(heights)*0.5))
```

Training and Test Sets

We can use the result of the `createDataPartition` function call to define the training and test sets like this:

```
test_set <- heights[test_index, ]
train_set <- heights[-test_index, ]
```

We develop an algorithm using **only** the training set. Once we are done developing the algorithm, we will **freeze** it and evaluate it using the test set. The simplest way to evaluate the algorithm when the outcomes are categorical is by simply reporting the proportion of cases that were correctly predicted in the test set. This metric is usually referred to as **overall accuracy**.

Overall Accuracy

To demonstrate the use of overall accuracy, we will build two competing algorithms and compare them.

Let's start by developing the simplest possible machine algorithm: guessing the outcome.

```
y_hat <- sample(c("Male", "Female"),
                length(test_index), replace = TRUE)
```

We are completely ignoring the predictor and simply guessing the sex.

Overall Accuracy

In machine learning applications, it is useful to use factors to represent the categorical outcomes because **R** functions developed for machine learning, such as those in the `caret` package, require or recommend that categorical outcomes be coded as factors. So convert `y_hat` to factors using the `factor` function:

```r
set.seed(2024)
y_hat <- sample(c("Male", "Female"),
                length(test_index), replace = TRUE) |>
  factor(levels = levels(test_set$sex))
```

Overall Accuracy

The *overall accuracy* is simply defined as the overall proportion that is predicted correctly:

```
mean(y_hat == test_set$sex)
```

```
## [1] 0.4819048
```

Not surprisingly, our accuracy is about 50%. We are guessing!

Overall Accuracy

Can we do better? Exploratory data analysis suggests we can because, on average, males are slightly taller than females:

```r
heights |>
  group_by(sex) |>
  summarize(means = mean(height), sds = sd(height))
```

```
## # A tibble: 2 x 3
##   sex    means   sds
##   <fct>  <dbl> <dbl>
## 1 Female  64.9  3.76
## 2 Male    69.3  3.61
```

Overall Accuracy

But how do we make use of this insight? Let's try another simple approach: predict `Male` if height is within two standard deviations from the average male:

```r
y_hat <- ifelse(x > 62, "Male", "Female") |>
  factor(levels = levels(test_set$sex))
```

The accuracy goes up from 0.50 to about 0.80:

```r
mean(y == y_hat)
```

```
## [1] 0.7933333
```

Overall Accuracy

But can we do even better? In the example above, we used a cutoff of 62, but we can examine the accuracy obtained for other cutoffs and then pick the value that provides the best results.

But remember, **it is important that we optimize the cutoff using only the training set**: the test set is only for evaluation.

Although for this simplistic example it is not much of a problem, later we will learn that evaluating an algorithm on the training set can lead to **overfitting**, which often results in dangerously over-optimistic assessments.

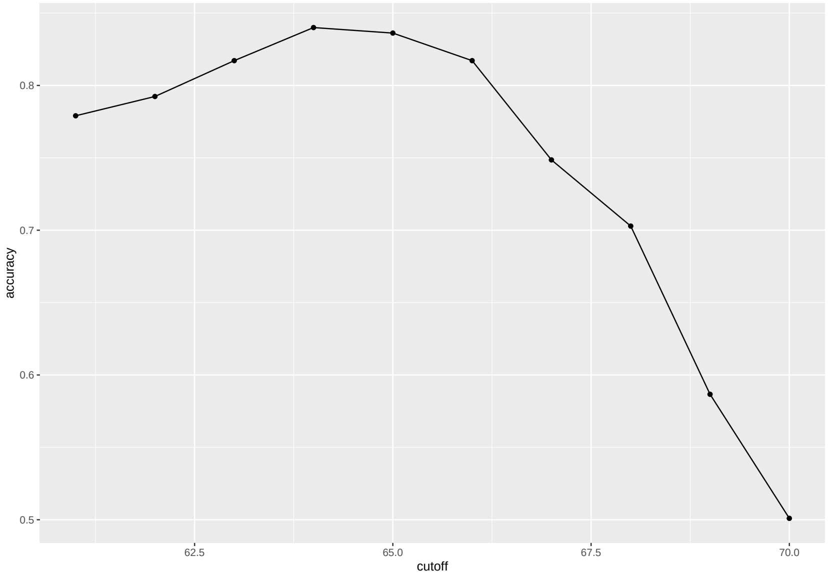
Overall Accuracy

Here we examine the accuracy of 10 different cutoffs and pick the one yielding the best result:

```r
cutoff <- seq(61, 70)
accuracy <- map_dbl(cutoff, function(x){
  y_hat <- ifelse(train_set$height > x, "Male", "Female") |>
    factor(levels = levels(test_set$sex))
  mean(y_hat == train_set$sex)
})
```

We can make a plot showing the accuracy obtained on the training set for males and females:

Overall Accuracy



Overall Accuracy

We see that the maximum value is:

```
max(accuracy)
```

```
## [1] 0.84
```

which is much higher than 0.5. The cutoff resulting in this accuracy is:

```
best_cutoff <- cutoff[which.max(accuracy)]
best_cutoff
```

```
## [1] 64
```

Overall Accuracy

We can now test this cutoff on our test set to make sure our accuracy is not overly optimistic:

```
y_hat <- ifelse(test_set$height > best_cutoff,"Male","Female") |>
  factor(levels = levels(test_set$sex))
mean(y_hat == test_set$sex)
```

```
## [1] 0.8133333
```

We see that it is a bit lower than the accuracy observed for the training set, but it is still better than guessing. And by testing on a dataset that we did not train on, we know our result is not due to cherry-picking a good result.

The Confusion Matrix

The prediction rule we developed in the previous section predicts `Male` if the student is taller than 64 inches. Given that the average female is about 64 inches, this prediction rule seems wrong. What happened? If a student is the height of the average female, shouldn't we predict `Female`?

The Confusion Matrix

Generally speaking, overall accuracy can be a deceptive measure. To see this, we will start by constructing what is referred to as the *confusion matrix*, which basically tabulates each combination of prediction and actual value. We can do this in **R** using the function `table`:

```r
table(predicted = y_hat, actual = test_set$sex)
```

```
##            actual
## predicted Female Male
##    Female     48   27
##    Male       71  379
```

The Confusion Matrix

If we study this table closely, it reveals a problem. If we compute the accuracy separately for each sex, we get:

```
test_set |>
  mutate(y_hat = y_hat) |>
  group_by(sex) |>
  summarize(accuracy = mean(y_hat == sex))
```

```
## # A tibble: 2 x 2
##   sex    accuracy
##   <fct>     <dbl>
## 1 Female    0.403
## 2 Male      0.933
```

The Confusion Matrix

There is an imbalance in the accuracy for males and females: too many females are predicted to be male. We are calling almost half of the females male! How can our overall accuracy be so high then? This is because the **prevalence** of males in this dataset is high. These heights were collected from three data sciences courses, two of which had more males enrolled:

```r
prev <- mean(y == "Male")
prev
```

```
## [1] 0.7733333
```

The Confusion Matrix

So when computing overall accuracy, the high percentage of mistakes made for females is outweighed by the gains in correct calls for men. **This can actually be a big problem in machine learning.** If your training data is biased in some way, you are likely to develop algorithms that are biased as well. The fact that we used a test set does not matter because it is also derived from the original biased dataset. This is one of the reasons we look at metrics other than overall accuracy when evaluating a machine learning algorithm.

The Confusion Matrix

There are several metrics that we can use to evaluate an algorithm in a way that prevalence does not cloud our assessment, and these can all be derived from the confusion matrix. A general improvement to using overall accuracy is to study **sensitivity** and **specificity** separately.

Sensitivity and Specificity

In general, **sensitivity** is defined as the ability of an algorithm to predict a positive outcome when the actual outcome is positive: $\hat{Y} = 1$ when $Y = 1$. Stated in terms of probability, this is
$P(\text{Predicted Positive}|\text{Actually Positive})$.

Because an algorithm that calls everything positive ($\hat{Y} = 1$ no matter what) has perfect sensitivity, this metric on its own is not enough to judge an algorithm.

Sensitivity and Specificity

For this reason, we also examine **specificity**, which is generally defined as the ability of an algorithm to not predict a positive $\hat{Y} = 0$ when the actual outcome is not a positive $Y = 0$. Stated in terms of probability, this is $P(\text{Predicted Negative}|\text{Actually Negative})$.

Sensitivity and Specificity

We name the four entries of the **confusion matrix**:

	Actually Positive	Actually Negative
Predicted positive	True positives (TP)	False positives (FP)
Predicted negative	False negatives (FN)	True negatives (TN)

Sensitivity and Specificity

Sensitivity is typically quantified by $TP/(TP + FN)$, the proportion of actual positives (the first column $= TP + FN$) that are called positives (TP). This quantity is also referred to as the **true positive rate** (TPR) or **recall**.

Specificity is defined as $TN/(TN + FP)$ or the proportion of negatives (the second column $= FP + TN$) that are called negatives (TN). This quantity is also called the **true negative rate** (TNR).

Sensitivity and Specificity

There is another way of quantifying accuracy which is $TP/(TP + FP)$ or the proportion of outcomes called positives (the first row or $TP + FP$) that are actually positives (TP). This quantity is referred to as **positive predictive value (PPV)** and also as **precision**. Note that, unlike TPR and TNR, precision depends on prevalence since higher prevalence implies you can get higher precision even when guessing.

Sensitivity and Specificity

The multiple names can be confusing, so we include a table to help us remember the terms. The table includes a column that shows the definition if we think of the proportions as probabilities.

Measure of	Name 1	Name 2	Definition	Prob. Representation
Sensitivity	TPR	Recall	$\frac{\text{TP}}{\text{TP}+\text{FN}}$	$P(\hat{Y}=1\|Y=1)$
Specificity	TNR	$1-$ FPR	$\frac{\text{TN}}{\text{TN}+\text{FP}}$	$P(\hat{Y}=0\|Y=0)$
Precision	PPV		$\frac{\text{TP}}{\text{TP}+\text{FP}}$	$P(Y=1\|\hat{Y}=1)$
	NPV		$\frac{\text{TN}}{\text{TN}+\text{FN}}$	$P(Y=0\|\hat{Y}=0)$

Here TPR is True Positive Rate, FPR is False Positive Rate, PPV is Positive Predictive Value, and NPV is Negative Predictive Value.

Sensitivity and Specificity

The caret function confusionMatrix computes all these metrics for us once we define what category "positive" is. The function expects factors as input, and the first level is considered the positive outcome or $Y = 1$. In our example, Female is the first level because it comes before Male alphabetically. If you type this into **R** you will see several metrics including accuracy, sensitivity, specificity, and PPV.

```
cm <- confusionMatrix(data = y_hat,
                      reference = test_set$sex)
cm$table
```

```
##           Reference
## Prediction Female Male
##     Female     48   27
##     Male       71  379
```

Sensitivity and specificity

You can acceess these directly, for example, like this:

```
cm$overall["Accuracy"]
```

```
##  Accuracy
## 0.8133333
```

```
cm$byClass[c("Sensitivity", "Specificity", "Prevalence")]
```

```
## Sensitivity Specificity  Prevalence
##   0.4033613   0.9334975   0.2266667
```

```
cm$byClass["Balanced Accuracy"]
```

```
## Balanced Accuracy
##         0.6684294
```

The balanced accuracy is calculated by taking the average of sensitivity and specificity.

Sensitivity and Specificity

We can see that the high overall accuracy is possible despite relatively low sensitivity. As we hinted at above, the reason this happens is because of the low prevalence (0.23): the proportion of females is low. Because prevalence is low, failing to predict actual females as females (low sensitivity) does not lower the accuracy as much as failing to predict actual males as males (low specificity).

Sensitivity and Specificity

Let's increase the cutoff to 67 inches.

```
y_hat2 <- ifelse(test_set$height > 67, "Male", "Female") |>
  factor()
cm2 <- confusionMatrix(data=y_hat2, reference=test_set$sex)
cm2$overall["Accuracy"]
```

```
##  Accuracy
## 0.7257143
```

```
cm2$byClass[c("Sensitivity","Specificity", "Prevalence")]
```

```
## Sensitivity Specificity  Prevalence
##   0.7226891   0.7266010   0.2266667
```

```
cm2$byClass["Balanced Accuracy"]
```

```
## Balanced Accuracy
##          0.724645
```

Section 2

Cross Validation with kNN Example

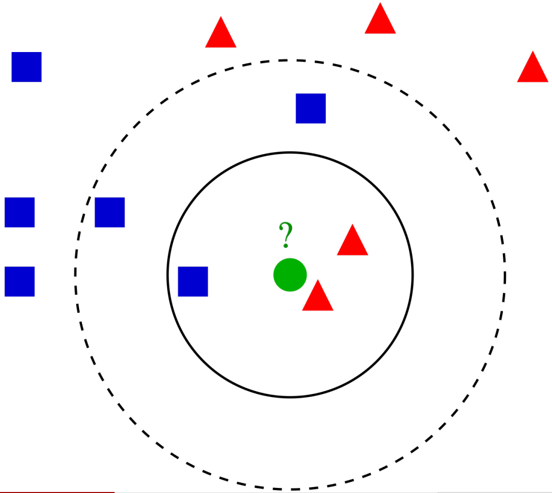
Cross Validation

In the previous example, we split our data into training and testing groups so as not to overfit and to get an idea of how the model works for new data.

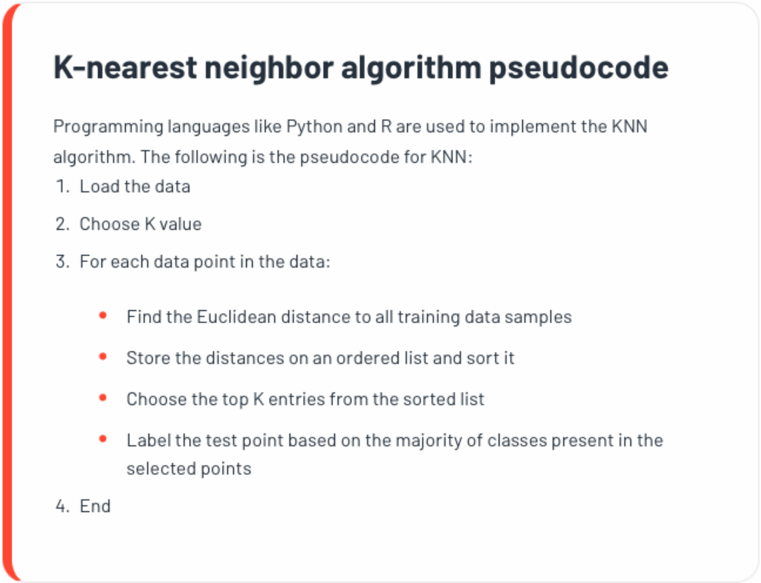
Cross-validation takes this one step forward. Cross-validation is one of the most important ideas in machine learning. Here we focus on the conceptual and mathematical aspects. We will describe how to implement cross validation in practice in later examples.

K-Nearest Neighbors (kNN)

To motivate the concept, we will introduce an actual machine learning algorithm: **k-nearest neighbors (kNN)**.



K-Nearest Neighbors (kNN)



K-nearest neighbor algorithm pseudocode

Programming languages like Python and R are used to implement the KNN algorithm. The following is the pseudocode for KNN:

1. Load the data
2. Choose K value
3. For each data point in the data:
   - Find the Euclidean distance to all training data samples
   - Store the distances on an ordered list and sort it
   - Choose the top K entries from the sorted list
   - Label the test point based on the majority of classes present in the selected points
4. End

K-Nearest Neighbors (kNN)

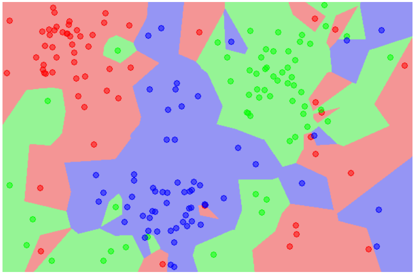
With k-nearest neighbors (kNN) we estimate the conditional probability function:

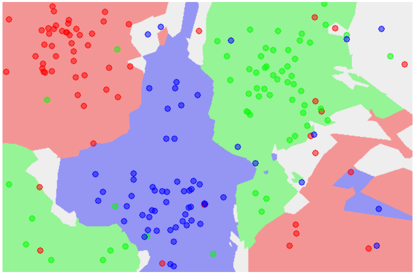
$$p(x_1, x_2) = \mathrm{P}(Y = 1 \mid X_1 = x_1, X_2 = x_2).$$

First we define the distance between each of the observations. Then, for any point (x_1, x_2) for which we want an estimate of $p(x_1, x_2)$, we look for the k nearest points to (x_1, x_2) and then take an average of the 0s and 1s associated with these points. We refer to the set of points used to compute the average as the *neighborhood*. This gives us an estimate $\hat{p}(x_1, x_2)$.

K-Nearest Neighbors (kNN)

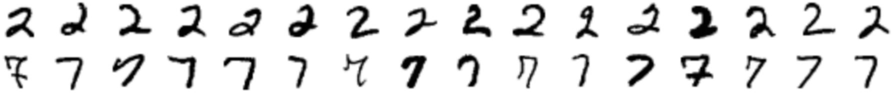
Using *k=1*: and *k*=5:





K-Nearest Neighbors (kNN): Example

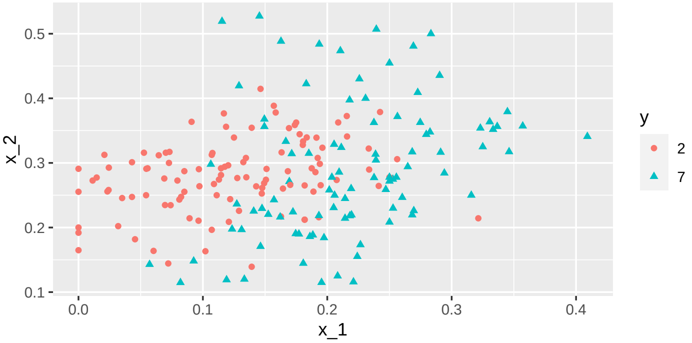
We will use the `mnist_27` data set in the `dslabs` package. This dataset contains information about predicting hand-written numbers. In this dataset, only 2's and 7's are considered. The data have already been split into a testing and training set. Each of these have three columns: `y`, `x_1`, and `x_2`. `y` is the true number, `x_1` is the proportion of dark pixels in the upper-left quadrant, and `x_2` is the proportion of dark pixels in the lower-right quadrant.



K-Nearest Neighbors (kNN): Example

Using this data set:

```
library(dslabs); data("mnist_27")
mnist_27$test |>
  ggplot(aes(x_1, x_2, color = y, shape = y)) +
    geom_point()
```



K-Nearest Neighbors (kNN): Example

We can use the knn3 function from the caret package as follows, with the number of neighbors equal to $k = 5$.:

```r
library(caret)
knn_fit <- knn3(y ~ ., data = mnist_27$train, k = 5)
```

Note that we have two classes here: a 2 or a 7. Therefore, we should use an odd number for k to avoid ties. If we had an odd number of classes, then an even number for k should be used.

K-Nearest Neighbors (kNN): Example

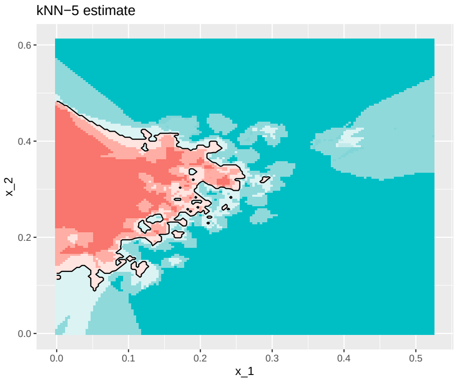
Since our data set is balanced (the prevalence is 0.53) and we care just as much about sensitivity as we do about specificity, we will use accuracy to quantify performance.

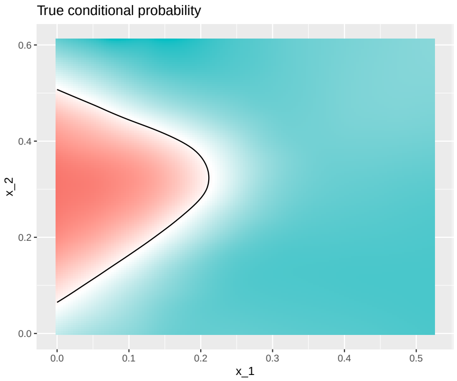
The `predict` function for `knn` produces a probability for each class.

```
y_hat_knn <- predict(knn_fit, mnist_27$test, type = "class")
confusionMatrix(y_hat_knn, mnist_27$test$y)$overall["Accuracy"]
```

```
## Accuracy
##    0.815
```

K-Nearest Neighbors (kNN): Example





Over-Training

Over-training or **over-fitting** results in having higher accuracy in the train set compared to the test set:

```
y_hat_knn <- predict(knn_fit, mnist_27$train, type = "class")
confusionMatrix(y_hat_knn, mnist_27$train$y)$overall["Accuracy"]
```

```
## Accuracy
##   0.8825
```

```
y_hat_knn <- predict(knn_fit, mnist_27$test, type = "class")
confusionMatrix(y_hat_knn, mnist_27$test$y)$overall["Accuracy"]
```

```
## Accuracy
##    0.815
```

Over-Training

Over-training is at its worst when we set $k = 1$:

```
knn_fit_1 <- knn3(y ~ ., data = mnist_27$train, k = 1)
y_hat_knn_1 <- predict(knn_fit_1, mnist_27$train, type = "class")
confusionMatrix(y_hat_knn_1, mnist_27$train$y)$overall["Accuracy"]
```

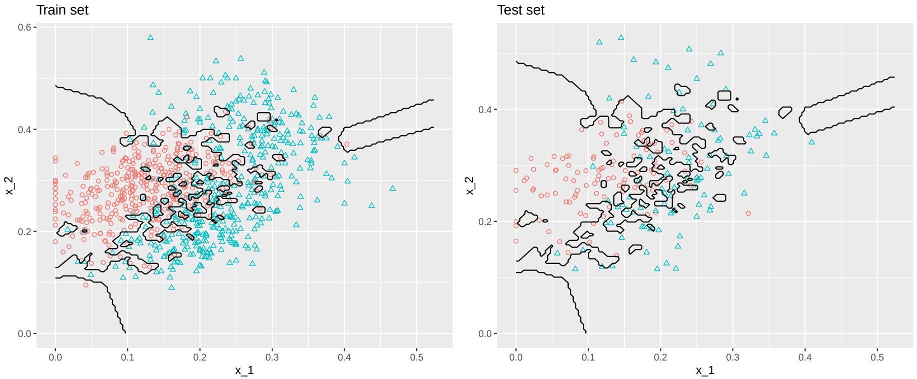
```
## Accuracy
##  0.99625
```

```
y_hat_knn_1 <- predict(knn_fit_1, mnist_27$test, type = "class")
confusionMatrix(y_hat_knn_1, mnist_27$test$y)$overall["Accuracy"]
```

```
## Accuracy
##     0.73
```

Over-Training

We can see the over-fitting problem in this figure.



Over-Smoothing

Although not as badly as with $k = 1$, we saw that $k = 5$ is also over-trained. Hence, we should consider a larger k. Let's try, as an example, a much larger number: $k = 401$.

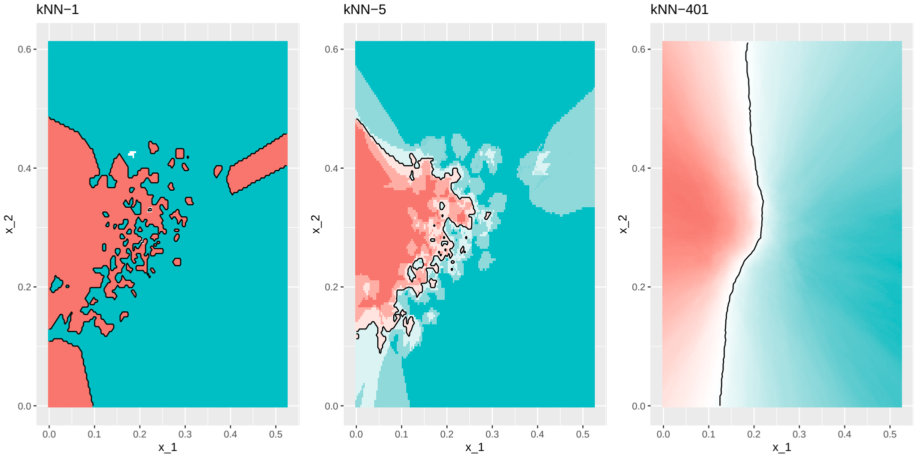
```
knn_fit_401 <- knn3(y ~ ., data = mnist_27$train, k = 401)
y_hat_knn_401 <- predict(knn_fit_401,mnist_27$train,type = "class")
confusionMatrix(y_hat_knn_401,mnist_27$train$y)$overall["Accuracy"]
```

```
## Accuracy
##  0.81375
```

```
y_hat_knn_401 <- predict(knn_fit_401,mnist_27$test,type = "class")
confusionMatrix(y_hat_knn_401, mnist_27$test$y)$overall["Accuracy"]
```

```
## Accuracy
##     0.79
```

Over-Smoothing



Picking the *k* in kNN

So how do we pick k? In principle, we want to pick the k that maximizes accuracy, or minimizes the expected MSE (defined later).

The goal of **cross validation** is to estimate these quantities for any given algorithm and set of tuning parameters such as k. To understand why we need a special method to do this let's repeat what we did above but for different values of k:

```
ks <- seq(3, 251, 2)
```

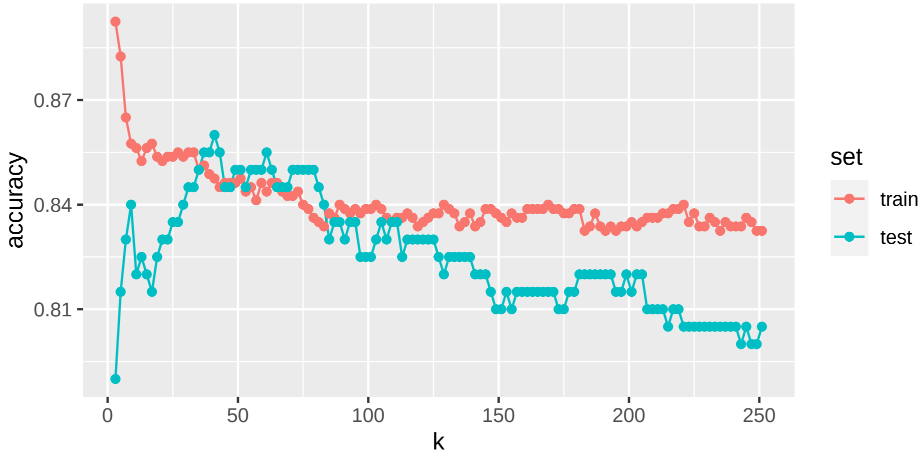
Picking the *k* in kNN

We do this using `map_df` function to repeat the function for each element of the vector.

```r
library(purrr)
accuracy <- map_df(ks, function(k){
  fit <- knn3(y ~ ., data = mnist_27$train, k = k)

  y_hat <- predict(fit, mnist_27$train, type = "class")
  cm_train <- confusionMatrix(y_hat, mnist_27$train$y)
  train_acc <- cm_train$overall["Accuracy"]

  y_hat <- predict(fit, mnist_27$test, type = "class")
  cm_test <- confusionMatrix(y_hat, mnist_27$test$y)
  test_acc <- cm_test$overall["Accuracy"]

  tibble(train = train_acc, test = test_acc)
})
```

Picking the k in kNN

Note that we estimate accuracy by using both the training set and the test set. We can now plot the accuracy estimates for each value of k:



Picking the k in kNN

If we were to use these estimates to pick the k that maximizes accuracy, we would use the estimates built on the test data:

```
ks[which.max(accuracy$test)]
```

```
## [1] 41
```

```
max(accuracy$test)
```

```
## [1] 0.86
```

Picking the k in kNN

First, note that the “best” estimate for k obtained for the training set is generally lower than the estimate obtained using the test set, with the difference larger for smaller values of k. This is due to over-training.

Also note that the accuracy versus k plot is quite jagged. We do not expect this because small changes in k should not affect the algorithm’s performance too much. The jaggedness is explained by the fact that the accuracy is computed on a sample and therefore is a random variable. This demonstrates why we prefer to minimize the expected, or average, loss (defined later) rather than the loss we observe with one dataset.

Picking the k in kNN

Another reason we need a better estimate of accuracy is that if we use the test set to pick this k, we should not expect the accompanying accuracy estimate to extrapolate to the real world. This is because even here <u>we broke a golden rule of machine learning</u>: we selected the k using the test set. Cross validation also provides an estimate that takes this into account.

Mathematical Description of Cross Validation

A common goal of machine learning is to find an algorithm that produces predictors $\hat{Y}$ for an outcome Y that minimizes the mean squared error (MSE):

$$\text{MSE} = \frac{1}{N}\sum_{i=1}^{N}(Y_i - \hat{Y}_i)^2$$

When all we have at our disposal is one data set, we can estimate the MSE with the observed MSE like this:

$$\hat{\text{MSE}} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

These two are often referred to as the *true error* and *apparent error*, respectively.

Mathematical Description of Cross Validation

There are two important characteristics of the apparent error we should always keep in mind:

1. Because our data is random, the apparent error is a random variable. For example, the dataset we have may be a random sample from a larger population. An algorithm may have a lower apparent error than another algorithm due to luck.
2. If we train an algorithm on the same dataset that we use to compute the apparent error, we might be overtraining. In general, when we do this, the apparent error will be an underestimate of the true error. We will see an extreme example of this with k-nearest neighbors.

Mathematical Description of Cross Validation

Cross validation is a technique that permits us to alleviate both these problems. To understand cross validation, it helps to think of the true error, a theoretical quantity, as the average of many apparent errors obtained by applying the algorithm to B new random samples of the data, none of them used to train the algorithm:

$$\frac{1}{B}\sum_{b=1}^{B}\frac{1}{n}\sum_{i=1}^{n}\left(y_i^b - \hat{y}_i^b\right)^2$$

with B a large number that can be thought of as practically infinite.

Mathematical Description of Cross Validation

As already mentioned, this is a theoretical quantity because we only have available one set of outcomes: $y_1, \ldots, y_n$. Cross validation is based on the idea of imitating the theoretical setup above as best we can with the data we have.

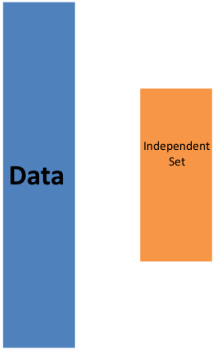
To do this, we have to generate a series of different random samples. There are several approaches we can use, but the general idea for all of them is to randomly generate smaller datasets that are not used for training, and instead used to estimate the true error.

Section 3

K-Fold Cross Validation

K-Fold Cross Validation

The first one we describe is **K-fold cross validation**. Note that his K is different than the k-nearest neighbors k value. A machine learning challenge starts with a data set (blue). We need to use this to build an algorithm that will be used in an independent validation data set (yellow).

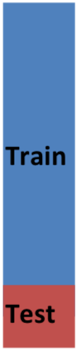


K-Fold Cross Validation

But we don't get to see these independent datasets.

K-Fold Cross Validation

So to imitate this situation, we carve out a piece of our dataset and pretend it is an independent dataset: we divide the dataset into a **training set** (blue) and a **test set** (red). We will train our algorithm exclusively on the training set and use the test set only for evaluation purposes.



K-Fold Cross Validation

We usually try to select a small piece of the data set so that we have as much data as possible to train. However, we also want the test set to be large so that we obtain a stable estimate of the loss without fitting an impractical number of models. Typical choices are to use 10%-20% of the data for testing.

K-Fold Cross Validation

Now this presents a new problem because for most machine learning algorithms we need to select parameters, for example the number of neighbors k in k-nearest neighbors. Here, we will refer to the set of parameters as $\boldsymbol{\lambda}$.

We need to optimize algorithm parameters without using our test set and we know that if we optimize and evaluate on the same dataset, we will overtrain.

For each set of algorithm parameters being considered, we want an estimate of the MSE and then we will choose the parameters with the smallest MSE. Cross validation provides this estimate.

K-Fold Cross Validation

First, before we start the cross validation procedure, it is important to fix all the algorithm parameters. We will use $\hat{y}_i(\boldsymbol{\lambda})$ to denote the predictors obtained when we use parameters $\boldsymbol{\lambda}$.

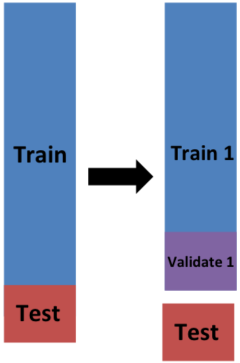
So, if we are going to imitate this definition:

$$\text{MSE}(\boldsymbol{\lambda}) = \frac{1}{B}\sum_{b=1}^{B}\frac{1}{n}\sum_{i=1}^{n}\left(y_i^b - \hat{y}_i^b(\boldsymbol{\lambda})\right)^2$$

We want to consider datasets that can be thought of as an independent random sample and we want to do this several times. With K-fold cross validation, we do it K times. We are showing an example that uses $K = 5$.

K-Fold Cross Validation

We will eventually end up with K samples, but let's start by describing how to construct the first: we simply pick $m = n/K$ observations at random (we round if m is not a round number) and think of these as a random sample $y_1^b, \ldots, y_m^b$, with $b = 1$. We call this the validation set:



K-Fold Cross Validation

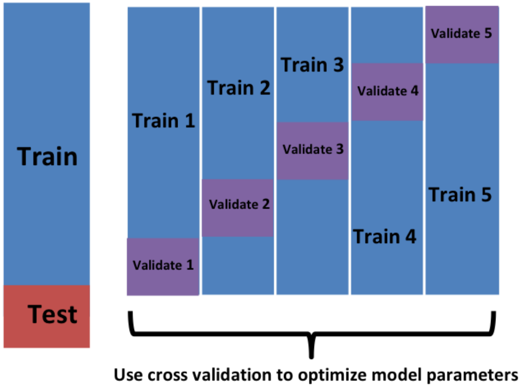
Now we can fit the model in the training set, then compute the apparent error on the validation set:

$$\hat{\text{MSE}}_b(\boldsymbol{\lambda}) = \frac{1}{m}\sum_{i=1}^{m}\left(y_i^b - \hat{y}_i^b(\boldsymbol{\lambda})\right)^2$$

Note: $n =$ sample size of training and testing data sets combined while $m =$ sample size of validation data set.

K-Fold Cross Validation

Note that this is just one sample and will therefore return a noisy estimate of the true error. This is why we take K samples, not just one. In K-fold cross validation, we randomly split the observations into K non-overlapping sets:



K-Fold Cross Validation

Now we repeat the calculation above for each of these sets $b = 1, \ldots, K$ and obtain $\hat{\text{MSE}}_1(\boldsymbol{\lambda}), \ldots, \hat{\text{MSE}}_K(\boldsymbol{\lambda})$. Then, for our final estimate, we compute the average:

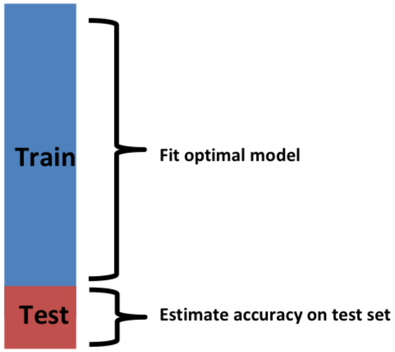
$$\hat{\text{MSE}}(\boldsymbol{\lambda}) = \frac{1}{B} \sum_{b=1}^{K} \hat{\text{MSE}}_b(\boldsymbol{\lambda}) = \frac{1}{B} \sum_{b=1}^{K} \left[\frac{1}{m} \sum_{i=1}^{m} \left(y_i^b - \hat{y}_i^b(\boldsymbol{\lambda}) \right)^2 \right]$$

and obtain an estimate of our loss.

The final step would be to select the $\boldsymbol{\lambda}$ that minimizes the MSE.

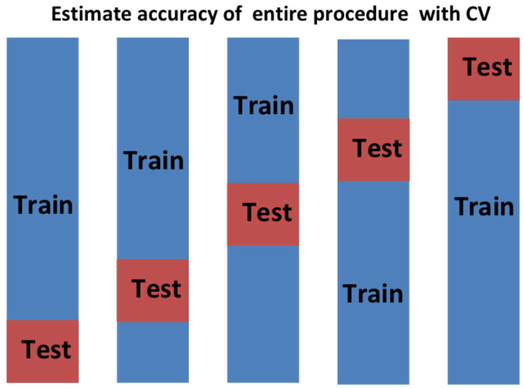
K-Fold Cross Validation

We have described how to use cross validation to optimize parameters. However, we now have to take into account the fact that the optimization occurred on the training data. Here is where we use the test set we separated early on:



K-Fold Cross Validation

We can do cross validation again:

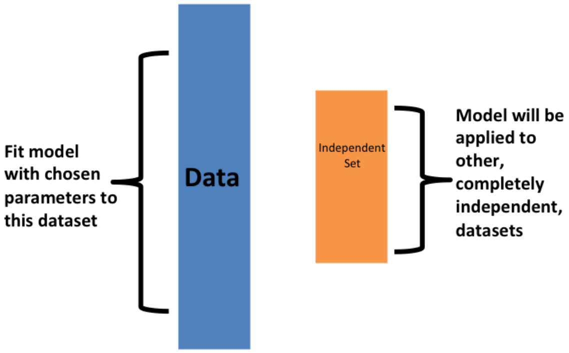


K-Fold Cross Validation

We can do cross validation multiple times to obtain a final estimate of our expected loss. However, note that this means that our entire computing time gets multiplied by K. You will soon learn that performing this task takes time because we are performing many complex computations. As a result, we are always looking for ways to reduce this time. For the final evaluation, we often just use the one test set.

Once we are satisfied with this model and want to make it available to others, we could refit the model on the entire dataset, without changing the optimized parameters.

K-Fold Cross Validation


Fit model with chosen parameters to this dataset
Data
Independent Set
Model will be applied to other, completely independent, datasets

K-Fold Cross Validation

Now how do we pick the cross validation K (not the k for kNN)? Large values of K are preferable because the training data better imitates the original dataset. However, larger values of K will have much slower computation time: for example, 100-fold cross validation will be 10 times slower than 10-fold cross validation. For this reason, the choices of $K = 5$ and $K = 10$ are popular.

K-Fold Cross Validation

One way we can improve the variance of our final estimate is to take more samples. To do this, we would no longer require the training set to be partitioned into non-overlapping sets. Instead, we would just pick K sets of some size at random.

K-Fold Cross Validation

One popular variation of this technique, at each fold, picks observations at random with replacement (which means the same observation can appear twice). This approach has some advantages (not discussed here) and is generally referred to as the *bootstrap*. In fact, this is the default approach in the **caret** package. We discussed bootstrapping in MATH 2140/3150, so we will not go over it again here.

Section 4

More on the `caret` Package

The caret Package

We have discussed the kNN machine learning algorithm. This is just one of many algorithms out there. Many of these algorithms are implemented in **R**. However, they are distributed via different packages, developed by different authors, and often use different syntax.

The caret Package

The **caret** (short for **C**lassification **A**nd **RE**gression **T**raining) package tries to consolidate these differences and provide consistency. It currently includes 238 different methods which are summarized in the **caret** package manual[1].

Keep in mind that **caret** does not include the needed packages and, to implement a package through **caret**, you still need to install the library. The required packages for each method are described in the package manual.

[1] https://topepo.github.io/caret/available-models.html

The caret train() functon

The **caret** package also provides a function that performs cross validation for us. Here we provide some examples showing how we use this incredibly helpful package. We will use the 2 or 7 example to illustrate:

```
library(tidyverse)
library(dslabs)
data("mnist_27")
```

The **caret** `train` function lets us train different algorithms using similar syntax. So, for example, we can type:

```
library(caret)
train_glm <- train(y ~ ., method = "glm", data = mnist_27$train)
train_knn <- train(y ~ ., method = "knn", data = mnist_27$train)
```

The caret train() functon

To make predictions, we can use the output of this function directly without needing to look at the specifics of `predict.glm` and `predict.knn`. Instead, we can learn how to obtain predictions from `predict.train`.

The code looks the same for both methods:

```
y_hat_glm <- predict(train_glm, mnist_27$test, type = "raw")
y_hat_knn <- predict(train_knn, mnist_27$test, type = "raw")
```

The caret train() Functon

This permits us to quickly compare the algorithms. For example, we can compare the accuracy like this:

```
confusionMatrix(y_hat_glm, mnist_27$test$y)$overall[["Accuracy"]]
```

```
## [1] 0.75
```

```
confusionMatrix(y_hat_knn, mnist_27$test$y)$overall[["Accuracy"]]
```

```
## [1] 0.84
```

Cross Validation

When an algorithm includes a tuning parameter, `train` automatically uses cross validation to decide among a few default values. To find out what parameter or parameters are optimized, you can read the manual [2] or study the output of:

```
getModelInfo("knn")
```

We can also use a quick lookup like this:

```
modelLookup("knn")
```

If we run it with default values:

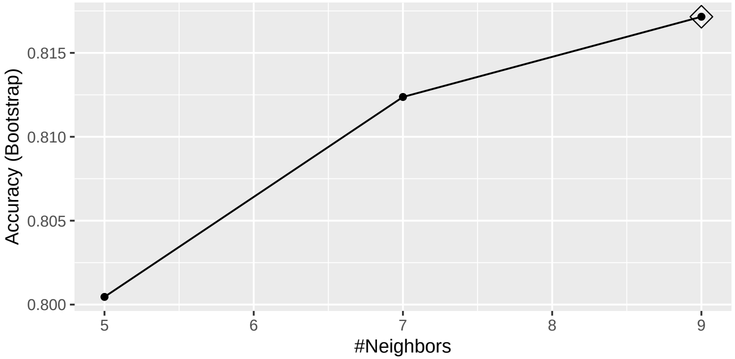
```
train_knn <- train(y ~ ., method = "knn", data = mnist_27$train)
```

[2] http://topepo.github.io/caret/available-models.html

Cross Validation

You can quickly see the results of the cross validation using the `ggplot` function. The argument `highlight` highlights the max:

```r
ggplot(train_knn, highlight = TRUE)
```



Cross Validation

By default, the cross validation is performed by taking 25 bootstrap samples comprised of 25% of the observations. We can change this to K-fold cross validation using the `trControl` option:
`trControl = trainControl(method = "cv", number = 10)`.
It does 10-fold cross validation by default if `number` is not specified.

For the `kNN` method, the default is to try $k = 5, 7, 9$. We change this using the `tuneGrid` parameter. The grid of values must be supplied by a data frame with the parameter names as specified in the `modelLookup` output.

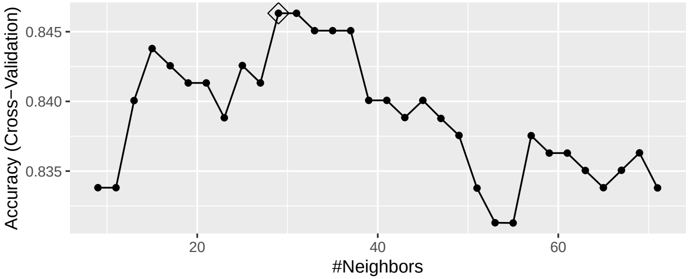
Here, we present an example where we try out 30 values between 9 and 67. To do this with **caret**, we need to define a column named `k`, so we use this:
`data.frame(k = seq(9, 67, 2))`.

Note that when running this code, we are fitting 30 versions of kNN to 25 bootstrapped samples. Since we are fitting $30 \times 25 = 750$ kNN models.

Cross Validation

We will set the seed because cross validation is a random procedure and we want to make sure the result here is reproducible.

```
set.seed(2024)
train_knn <- train(y ~ ., method = "knn",
                   data = mnist_27$train,
                   trControl = trainControl(method = "cv"),
                   tuneGrid = data.frame(k = seq(9, 71, 2)))
ggplot(train_knn, highlight = TRUE)
```



Cross Validation

To access the parameter that maximized the accuracy, you can use this:

```
train_knn$bestTune
```

```
##     k
## 11 29
```

and the best performing model like this:

```
train_knn$finalModel
```

```
## 29-nearest neighbor model
## Training set outcome distribution:
##
##   2   7
## 379 421
```

Cross Validation

The function `predict` will use this best performing model. Here is the accuracy of the best model when applied to the test set, which we have not used at all yet because the cross validation was done on the training set:

```r
confusionMatrix(predict(train_knn, mnist_27$test, type = "raw"),
                mnist_27$test$y)$overall["Accuracy"]
```

```
## Accuracy
##     0.84
```

Cross Validation

The results component of the train output includes several summary statistics related to the variability of the cross validation estimates:

```r
names(train_knn$results)
```

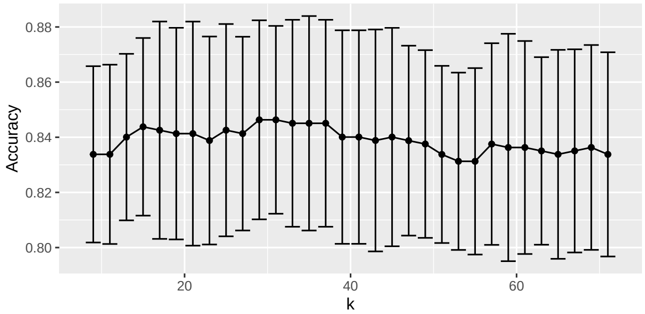
```
## [1] "k"          "Accuracy"   "Kappa"      "AccuracySD"
## [5] "KappaSD"
```

Note: Kappa is Cohen's Kappa and it is like classification accuracy, except that it is normalized at the baseline of random chance on your dataset. It is a more useful measure to use on problems that have an imbalance in the classes

Cross Validation

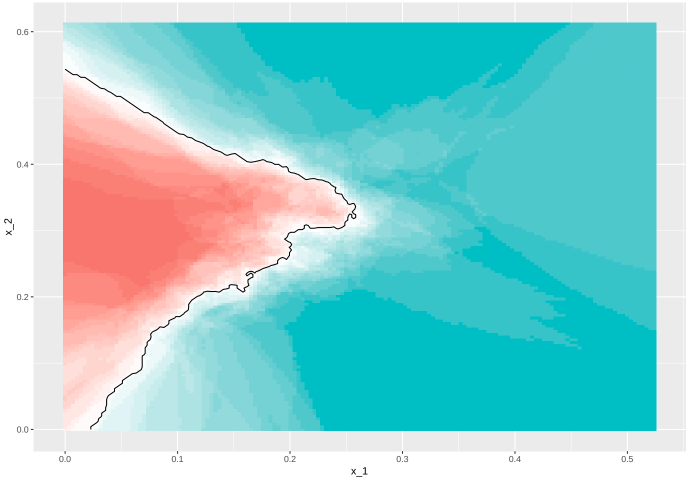
We can also see the standard deviation bars obtained from the cross validation samples. These are not confidence intervals.

```r
train_knn$results |>
  ggplot(aes(x = k, y = Accuracy)) +
  geom_line() + geom_point() +
  geom_errorbar(aes(x = k,
                    ymin = Accuracy - AccuracySD,
                    ymax = Accuracy + AccuracySD))
```



Example: Fitting with Loess

The best fitting kNN model approximates the true conditional probability:



Example: Fitting with Loess

However, we do see that the boundary is somewhat wiggly. This is because kNN, like the basic bin smoother, does not use a kernel. Kernels can be used to make a smoother line since they are based on models instead of just the empirical data.

To improve this we could try using a loess kernel. By reading through the available models part of the manual[3] we see that we can use the `gamLoess` method. In the manual[4] we also see that we need to install the **gam** package if we have not done so already:

```
install.packages("gam")
```

[3] https://topepo.github.io/caret/available-models.html

[4] https://topepo.github.io/caret/train-models-by-tag.html

Example: Fitting with Loess

Then we see that we have two parameters to optimize:

```
modelLookup("gamLoess")
```

```
##      model parameter  label forReg forClass probModel
## 1 gamLoess      span   Span   TRUE     TRUE      TRUE
## 2 gamLoess    degree Degree   TRUE     TRUE      TRUE
```

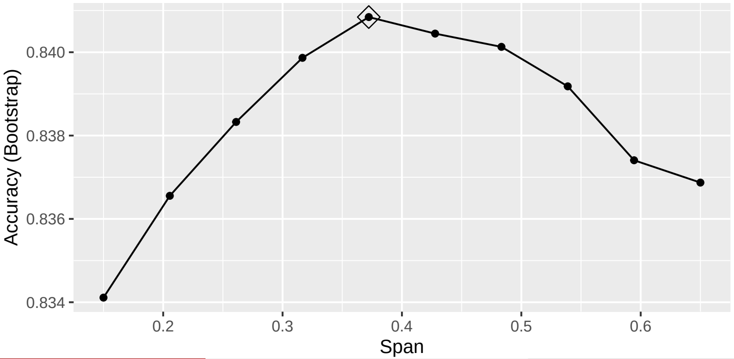
We will stick to a degree of 1. But to try out different values for the span, we still have to include a column in the table with the name `degree` so we can do this:

```
grid <- expand.grid(span = seq(0.15, 0.65, length = 10),
                    degree = 1)
```

Example: Fitting with Loess

We will use the default cross validation control parameters.

```
set.seed(2024)
train_loess <- train(y ~ ., method = "gamLoess",
                     tuneGrid = grid,
                     data = mnist_27$train)
ggplot(train_loess, highlight = TRUE)
```



Example: Fitting with Loess

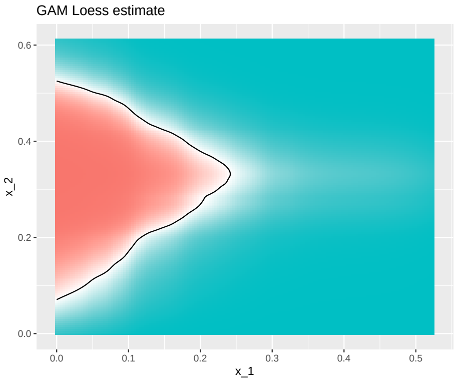
We can see that the method performs similar to kNN:

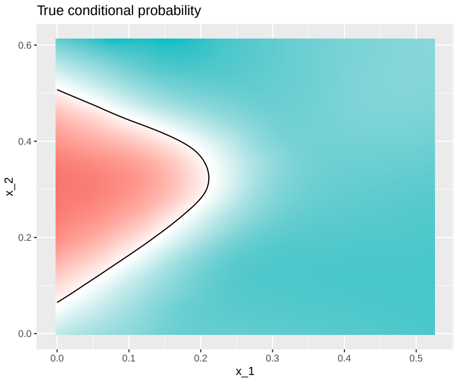
```
confusionMatrix(data = predict(train_loess, mnist_27$test),
                reference = mnist_27$test$y)$overall["Accuracy"]
```

```
## Accuracy
##     0.85
```

Example: Fitting with Loess

It produces a smoother estimate of the conditional probability, which, although not at all necessary, is a bit more aesthetically pleasing:





Conclusion

Many algorithms in statistical and machine learning rely on cross validation and/or other similar verification methods. We will continue to see this used as we continue in the course.

Session Info

```r
sessionInfo()
```

```
## R version 4.3.2 (2023-10-31)
## Platform: aarch64-apple-darwin20 (64-bit)
## Running under: macOS Sonoma 14.2.1
##
## Matrix products: default
## BLAS:   /Library/Frameworks/R.framework/Versions/4.3-arm64/Resources/lib/libRblas.0.dylib
## LAPACK: /Library/Frameworks/R.framework/Versions/4.3-arm64/Resources/lib/libRlapack.dylib;  LAPACK version 3
##
## locale:
## [1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
##
## time zone: America/Denver
## tzcode source: internal
##
## attached base packages:
## [1] splines   stats     graphics  grDevices utils
## [6] datasets  methods   base
##
## other attached packages:
##  [1] gam_1.22-3      foreach_1.5.2   gridExtra_2.3
##  [4] dslabs_0.7.6    caret_6.0-94    lattice_0.21-9
##  [7] lubridate_1.9.3 forcats_1.0.0   stringr_1.5.1
## [10] dplyr_1.1.4     purrr_1.0.2     readr_2.1.5
## [13] tidyr_1.3.0     tibble_3.2.1    ggplot2_3.4.4
## [16] tidyverse_2.0.0
##
## loaded via a namespace (and not attached):
##  [1] tidyselect_1.2.0     viridisLite_0.4.2
##  [3] timeDate_4022.108    farver_2.1.1
##  [5] fastmap_1.1.1        pROC_1.18.5
##  [7] digest_0.6.34        rpart_4.1.21
```