Lecture 5: Functions and Basic Classification Methods.

STAT GR5206 *Statistical Computing & Introduction to Data Science*

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October 5, 2018

Last Time

- **Character Data in** `R`. Commands like `nchar()`, `paste()`, `strsplit()`, `substr()`, `grep()`.
- **Regular Expressions**. A grammar (lots of rules) to works with patterns of characters.
- **Web Scraping**. Data from the internet.

Section I

Functions

Functions in R

Why Functions?

- Data structures tie related values into one object.
- Functions tie related commands into one object.
- Both cases: easier to understand, work with, and to build into larger structures.

Functions in R

Basic Structure

```
function_name <- function(arg1, arg2, ... ) {
  statements
  return(object)
}
```

Functions in R

Basic Structure

```
function_name <- function(arg1, arg2, ... ) {
  statements
  return(object)
}
```

- A **function** is a group of instructions that takes inputs, uses them to compute other values, and returns a result.
- We can write and add our own functions in R.
- Functions:
  1. Have names.
  2. *Usually* take in arguments.
  3. Include body of code that does something.
  4. *Usually* return an object at the end.

Example Function

A Function to Check for Significance at $\alpha = 0.05$

```
> # Input x should be a single p-value in [0,1]
> significant <- function(x) {
+   if (x <= 0.05) { return(TRUE) }
+   else { return(FALSE) }
+ }
```

Example Function

A Function to Check for Significance at $\alpha = 0.05$

```
> # Input x should be a single p-value in [0,1]
> significant <- function(x) {
+   if (x <= 0.05) { return(TRUE) }
+   else { return(FALSE) }
+ }
```

- First, tell `R` to define a function named `significant`.
- Brackets `{` and `}` mark the start and close of the body.
- `R` tells you you're in the body of the function by using $+$ as a prompt (instead of $>$).
- At the end, use the `return()` command.

Example Function

A ‘Robust’ Loss Function (for Outlier-Resistant Regression)

```
> # Inputs:  A vector of numbers (x)
> # Outputs: A loss vector with x^2 for small elements,
> #          and 2|x|-1 for large ones
>
> res_loss <- function(x) {
+   loss_vec <- ifelse(x^2 > 1, 2*abs(x) - 1, x^2)
+   return(loss_vec)
+ }
```

Example Function

A 'Robust' Loss Function (for Outlier-Resistant Regression)

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> # Inputs:  A vector of numbers (x)
> # Outputs: A loss vector with x^2 for small elements,
> #          and 2|x|-1 for large ones
>
> res_loss <- function(x) {
+   loss_vec <- ifelse(x^2 > 1, 2*abs(x) - 1, x^2)
+   return(loss_vec)
+ }
```

Let's try it:

```
> vec <- c(-0.5, 0.9, -3, 4)
> res_loss(vec)
```

```
[1] 0.25 0.81 5.00 7.00
```

Example Function

A ‘Robust’ Loss Function (for Outlier-Resistant Regression)

```
> res_loss <- function(x) {
+   loss_vec <- ifelse(x^2 > 1, 2*abs(x) - 1, x^2)
+   return(loss_vec)
+ }
```

Break apart the function

What are the...

- Inputs?
- Outputs?
- Body Statements?

Example Function

A ‘Robust’ Loss Function (for Outlier-Resistant Regression)

```
> res_loss <- function(x) {
+   loss_vec <- ifelse(x^2 > 1, 2*abs(x) - 1, x^2)
+   return(loss_vec)
+ }
```

Break apart the function

What are the...

- Inputs? `x`
- Outputs? `loss_vec`
- Body Statements?

```
loss_vec <- ifelse(x^2 > 1, 2*abs(x) - 1, x^2)
return(loss_vec)
```

When Should We Make a Function?

- Things you will rerun.
- Chunks of code that are small parts of bigger analyses.

Check Yourself

Task

Write a function called `FiveTimesSum` that takes as input a vector of numerical values and returns 5 times the sum of those values. Test it on the vector `1:3`. Your output should be 30.

Check Yourself

Task

Write a function called `FiveTimesSum` that takes as input a vector of numerical values and returns 5 times the sum of those values. Test it on the vector `1:3`. Your output should be 30.

Solution

```
> FiveTimesSum <- function(vec){
+   return(5*sum(vec))
+ }
> FiveTimesSum(1:3)
```

```
[1] 30
```

Named and Default Arguments

A 'Robust' Loss Function (for Outlier-Resistant Regression)

```
> # Inputs: A vector of numbers (x),
> #         crossover location (c > 0)
> # Outputs: A loss vector with x^2 for small elements,
> #          and 2*sqrt(c)*|x|-c for large ones
>
> res_loss2 <- function(x, c = 1) {
+   loss_vec <- ifelse(x^2 > c, 2*sqrt(c)*abs(x) - c, x^2)
+   return(loss_vec)
+ }
```

Named and Default Arguments

A 'Robust' Loss Function (for Outlier-Resistant Regression)

```
> # Inputs: A vector of numbers (x),
> #         crossover location (c > 0)
> # Outputs: A loss vector with x^2 for small elements,
> #          and 2*sqrt(c)*|x|-c for large ones
>
> res_loss2 <- function(x, c = 1) {
+   loss_vec <- ifelse(x^2 > c, 2*sqrt(c)*abs(x) - c, x^2)
+   return(loss_vec)
+ }
```

Let's try it:

```
> identical(res_loss(vec), res_loss2(vec, c=1))
```

```
[1] TRUE
```

Named and Default Arguments

A ‘Robust’ Loss Function (for Outlier-Resistant Regression)

```
> # Inputs: A vector of numbers (x),
> #         crossover location (c > 0)
> # Outputs: A loss vector with x^2 for small elements,
> #          and 2*sqrt(c)*|x|-c for large ones
>
> res_loss2 <- function(x, c = 1) {
+   loss_vec <- ifelse(x^2 > c, 2*sqrt(c)*abs(x) - c, x^2)
+   return(loss_vec)
+ }
```

Let’s try it:

```
> identical(res_loss(vec), res_loss2(vec, c=2))
```

```
[1] FALSE
```

Named and Default Arguments

Default values get used if names are missing:

```
> identical(res_loss2(vec, c=1), res_loss2(vec))
```

```
[1] TRUE
```

Named and Default Arguments

Default values get used if names are missing:

```
> identical(res_loss2(vec, c=1), res_loss2(vec))
```

```
[1] TRUE
```

Named argument can go in any order when they are explicitly tagged:

```
> identical(res_loss2(x=vec, c=2), res_loss2(c=2, x=vec))
```

```
[1] TRUE
```

Checking Arguments

Funny things can happen when arguments aren't as we expect:

```
> vec <- c(-0.5, 0.9, -3, 4)
> res_loss2(vec, c = c(1,1,1,5))
```

```
[1]  0.25000  0.81000  5.00000 12.88854
```

Checking Arguments

Funny things can happen when arguments aren't as we expect:

```
> vec <- c(-0.5, 0.9, -3, 4)
> res_loss2(vec, c = c(1,1,1,5))
```

```
[1]  0.25000  0.81000  5.00000 12.88854
```

```
> res_loss2(vec, c = -1)
```

```
[1] NaN NaN NaN NaN
```

Checking Arguments

Solution: Add some checks to your function.

A 'Robust' Loss Function (for Outlier-Resistant Regression)

```
> res_loss2 <- function(x, c = 1) {
+   # Scale should be a single positive number
+   stopifnot(length(c) == 1, c > 0)
+   loss_vec <- ifelse(x^2 > c, 2*sqrt(c)*abs(x) - c, x^2)
+   return(loss_vec)
+ }
```

Checking Arguments

Solution: Add some checks to your function.

A 'Robust' Loss Function (for Outlier-Resistant Regression)

```
> res_loss2 <- function(x, c = 1) {
+   # Scale should be a single positive number
+   stopifnot(length(c) == 1, c > 0)
+   loss_vec <- ifelse(x^2 > c, 2*sqrt(c)*abs(x) - c, x^2)
+   return(loss_vec)
+ }
```

`stopifnot()`

- Arguments are a series of expressions which should all be `TRUE`.
- Execution stops with error at first `FALSE`.

Checking Arguments

Solution: Add some checks to your function.

A 'Robust' Loss Function (for Outlier-Resistant Regression)

```
> res_loss2 <- function(x, c = 1) {
+   # Scale should be a single positive number
+   stopifnot(length(c) == 1, c > 0)
+   loss_vec <- ifelse(x^2 > c, 2*sqrt(c)*abs(x) - c, x^2)
+   return(loss_vec)
+ }
```

Test it:

```
> # res_loss2(vec, c = c(1,1,1,5))
> # res_loss2(vec, c = -1)
```

Check Yourself

Task

Write a function called `KTimesSum` that takes as input a vector of numerical values and a scalar value K (with a default value of 5). The function should return the sum of those values multiplied times the value K. Test it with the following: `KTimesSum(1:3)` and `KTimesSum(1:3, K = 10)`.

Check Yourself

Task

Write a function called `KTimesSum` that takes as input a vector of numerical values and a scalar value K (with a default value of 5). The function should return the sum of those values multiplied times the value K. Test it with the following: `KTimesSum(1:3)` and `KTimesSum(1:3, K = 10)`.

Solution

```
> KTimesSum <- function(vec, K = 5){
+   return(K*sum(vec))
+ }
> KTimesSum(1:3); KTimesSum(1:3, K = 10)
```

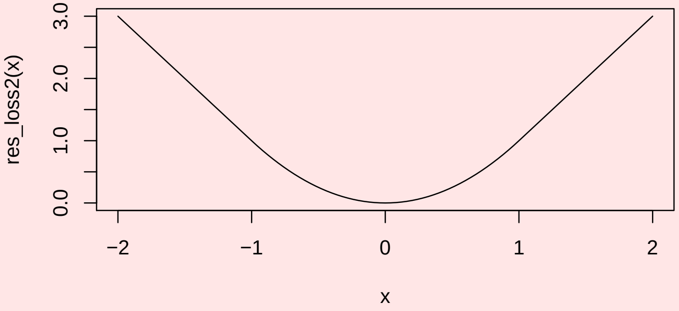
```
[1] 30
```

```
[1] 60
```

Use Your Functions in Other Functions

- Use your own function in built-in R functions like `apply()`.
- Ex: `curve(expression, from = , to = )` plots a curve.

```
> curve(res_loss2, from = -2, to = 2)
```



The R Environment

- The **global environment** (or the workspace) in R consists of the collection of your named objects.
- When you start an R session, a new environment is initialized (unless you load a saved environment).
- When a function is called, a new **local environment** is created within the body of the function.

Clearing the Global Environment

Note the code `rm(list=ls())` clears the R global environment.

The R Environment

Code Example.

The Function Environment

- Each function has its own (internal) **environment**.
- Names in the function environment override names from the **global environment**.
- Assignments in the internal environment don't change the global environment.
- Functions search for named variables (undefined in the function itself) in the environment in which the function was created (in our case, the global environment).

The Function Environment

```
> x <- 7
> y <- c("dog", "cat")
> addition <- function(y) {x <- x + y; return(x)}
> addition(1)
```

```
[1] 8
```

The Function Environment

```
> x <- 7
> y <- c("dog", "cat")
> addition <- function(y) {x <- x + y; return(x)}
> addition(1)
```

```
[1] 8
```

```
> x
```

```
[1] 7
```

```
> y
```

```
[1] "dog" "cat"
```

The Function Environment

```
> circle.area <- function(r) {return(pi*r^2)}
> circle.area(1:3)
```

```
[1]  3.141593 12.566371 28.274334
```

The Function Environment

```
> circle.area <- function(r) {return(pi*r^2)}
> circle.area(1:3)
```

```
[1]  3.141593 12.566371 28.274334
```

```
> true.pi <- pi # Save the real value
> pi      <- 3 # Assign a new value
> circle.area(1:3)
```

```
[1]  3 12 27
```

The Function Environment

```
> circle.area <- function(r) {return(pi*r^2)}
> circle.area(1:3)
```

```
[1]  3.141593 12.566371 28.274334
```

```
> true.pi <- pi # Save the real value
> pi      <- 3 # Assign a new value
> circle.area(1:3)
```

```
[1]  3 12 27
```

```
> pi <- true.pi # Restore the real value
> circle.area(1:3)
```

```
[1]  3.141593 12.566371 28.274334
```

Use Your Function Interfaces

The function **interfaces** are the places where the function interacts with the global environment: at the **inputs** and the **outputs**.

Use Your Function Interfaces

The function **interfaces** are the places where the function interacts with the global environment: at the **inputs** and the **outputs**.

- Interact with the rest of the system only at the interfaces:
  - Arguments should give your function all the information it needs
  - Reduces the risk of bugs
  - Exception would be universal constants like `pi`.
- Output should be only through `return()`.

Extended Example: Fitting a Model

The Model

We study the following idea: bigger cities tend to produce more economically per capita.

Geoffrey West et al.

A proposed statistical model for this relationship:

$$Y = \beta_0 X^{\beta_1} + \epsilon,$$

where

- Y: per-capita ‘gross metropolitan product’ of a city,
- X: is the population of the city,
- β_0, β_1: parameters,
- ϵ: noise.

The Data

```
> gmp <- read.table("gmp.txt", as.is = TRUE, header = TRUE)
> head(gmp)[1:3, ]
```

```
         city        gmp pcgmp
1 Abilene, TX 3.8870e+09 24490
2   Akron, OH 2.2998e+10 32889
3  Albany, GA 3.9550e+09 24269
```

The Data

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> gmp <- read.table("gmp.txt", as.is = TRUE, header = TRUE)
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          city        gmp pcgmp
1 Abilene, TX 3.8870e+09 24490
2   Akron, OH 2.2998e+10 32889
3  Albany, GA 3.9550e+09 24269
```

Variables

- city
- gmp: gross metropolitan product (money the city makes)
- pcgmp: per-capita gross metropolitan product (money the city makes divided by the number of people in the city)

The Data (cont.)

Our model uses the population, so let's create a variable for that in the dataset.

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$$\text{pcgmp} = \frac{\text{gmp}}{\text{population}} \quad \rightarrow \quad \text{population} = \frac{\text{gmp}}{\text{pcgmp}}.$$

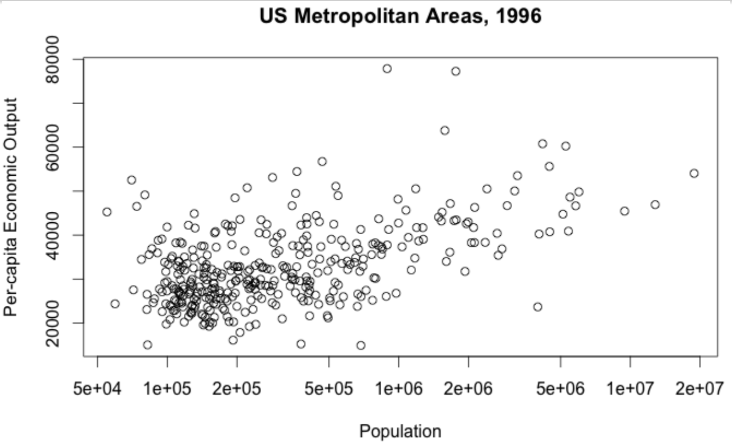
```
> gmp$pop <- gmp$gmp/gmp$pcgmp
> head(gmp)[1:3, ]
```

```
         city         gmp pcgmp      pop
1 Abilene, TX 3.8870e+09 24490 158717.8
2   Akron, OH 2.2998e+10 32889 699261.2
3  Albany, GA 3.9550e+09 24269 162965.1
```

The Data (cont)

Plotting Per-Capita GMP vs. Population

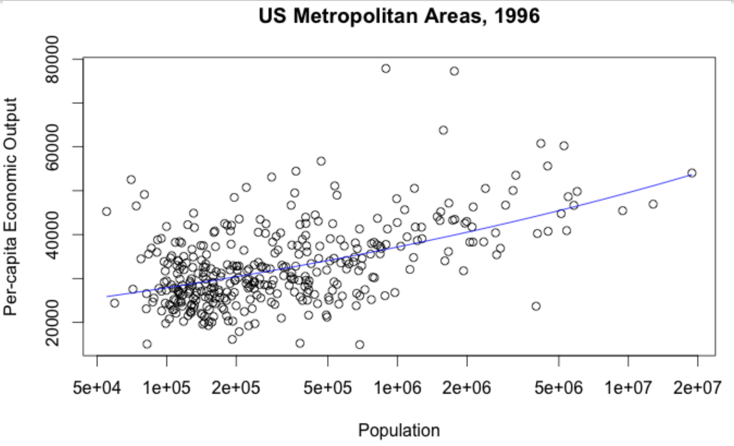
```
> plot(gmp$pop, gmp$pcgmp, log = "x", xlab = "Population",
+       ylab = "Per-capita Economic Output")
```



The Data (cont)

Plotting Per-Capita GMP vs. Population

```
> # beta_0 = 6611; beta_1 = 1/8
> curve(6611*x^{1/8}, add = TRUE, col = "blue")
```



Fitting the Function

Want to fit the model:

$$Y = 6611X^{\beta_1} + \epsilon.$$

We're assuming $\beta_0 = 6611$ and trying to estimate β_1 using the data.

Fitting the Function

Want to fit the model:

$$Y = 6611X^{\beta_1} + \epsilon.$$

We're assuming $\beta_0 = 6611$ and trying to estimate β_1 using the data.

Strategy

Minimize the sum of the squares!

$$\min_{\beta} \sum_{i=1}^{n} (Y_i - 6611X_i^{\beta})^2$$

where n is the number of data points.

Note this is the **training mean square error** (times n).

Optimizing a Function

Want to find $\min_x f(x)$.

Numerical Methods for Optimization

All numerical minimization methods perform roughly the same steps:

- Start with some point x_0.
- Find a sequence $x_0, x_1, \ldots, x_m$ such that $f(x_m)$ is a minimum.
- At a given point x_n, compute properties of f (such as $f'(x_n)$ and $f''(x_n)$).
- Based on these values, choose the next point x_{n+1}.

Optimizing a Function

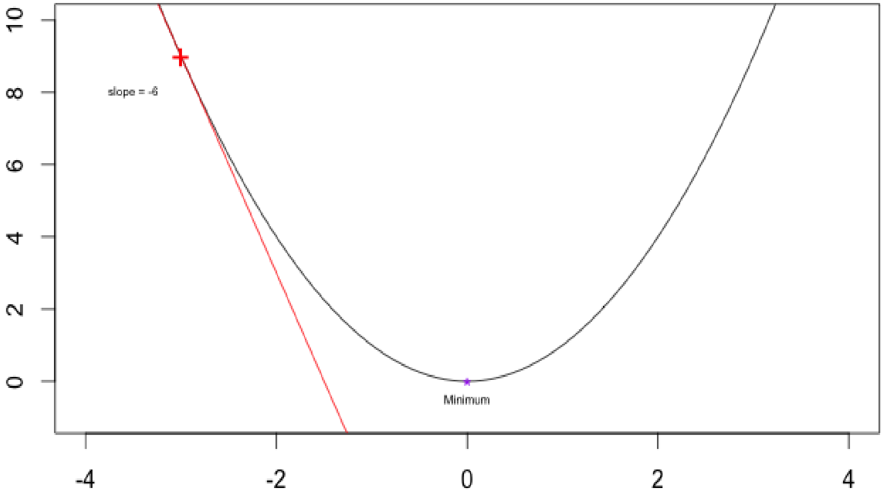
Gradient Descent is an iterative algorithm to find a (local) minimum of a function.

Gradient Descent

Procedure:

- Start at a point x_0
- Calculate the derivative at the point, $f'(x_0)$.
- Take a step in the opposite direction of the derivative to find x_1.
- Repeat.
- Stop when the derivative is small enough or at some set number of iterations.

Optimizing a Function



Fitting Our Function

Strategy

Minimize the sum of the squares!

$$\min_{\beta} \sum_{i=1}^{n} (Y_i - 6611 X_i^{\beta})^2.$$

In our example,

Initial point β_0. Approximate the derivative w.r.t. β and move in the opposite direction:

$$SSE(\beta_0) = \sum_{i=1}^{n} (Y_i - 6611 X_i^{\beta_0})^2$$

$$SSE'(\beta_0) \approx \frac{SSE(\beta_0 + h) - SSE(\beta_0)}{h} \quad \text{h is small}$$

$$\beta_1 \approx \beta_0 - c * SSE'(\beta_0) \quad \text{c scales our step size}$$

Fitting Our Function

$$SSE(\beta_0) = \sum_{i=1}^{n}(Y_i - 6611X_i^{\beta_0})^2$$

$$SSE'(\beta_0) \approx \frac{SSE(\beta_0 + h) - SSE(\beta_0)}{h}$$ h is small

$$\beta_1 \approx \beta_0 - c * SSE'(\beta_0)$$ c scales our step size

A first attempt at code:

```
> # Parameters
> max.iter          <- 100      # How long we run the alg.
> stop.deriv        <- 1/100    # If derivative is small, stop
> derivative.step   <- 1/1000   # This is h
> step.scale        <- 1e-15    # This is c
> # Initializations
> iter              <- 0        # Compare to max.iteration
> deriv             <- Inf      # Compare to stop.deriv
> beta              <- 0.15
```

A first attempt at code:

```
> max.iter    <- 100    # How long we run the alg.
> stop.deriv  <- 1/100  # If derivative is small, stop
> deriv.step  <- 1/1000 # This is h
> step.scale  <- 1e-15  # This is c
> iter        <- 0      # Iteration counter
> deriv       <- Inf
> beta        <- 0.15
> while((iter < max.iter) & (deriv > stop.deriv)) {
+   iter  <- iter + 1
+   sse.1 <- sum((gmp$pcgmp - 6611*gmp$pop^beta)^2)
+   sse.2 <- sum((gmp$pcgmp
+                  - 6611*gmp$pop^(beta + deriv.step))^2)
+   deriv <- (sse.2 - sse.1)/deriv.step
+   beta  <- beta - step.scale*deriv
+ }
> list(beta = beta, iteration = iter,
+      converged = (iter < max.iter))
```

A first attempt at code:

```
> list(beta = beta, iteration = iter,
+      converged = (iter < max.iter))
```

```
$beta
[1] 0.1258166

$iteration
[1] 100

$converged
[1] FALSE
```

What's Wrong With the Previous Attempt?

- **Not encapsulated**: Re-run by copying and pasting. Note easy to fit into bigger project.
- **Inflexible**: To edit initializations must copy, paste, re-run
- **Error-prone**: If you change the dataset, not sure if it would still work...
- **Hard to fix**: Should stop when *absolute value* of derivative is small.

First Fix

```
> est.scaling.exponent <- function(beta) {
+   max.iter      <- 100    # How long we run the alg.
+   stop.deriv    <- 1/100  # If derivative is small, stop
+   deriv.step    <- 1/1000 # This is h
+   step.scale    <- 1e-15  # This is c
+   iter          <- 0
+   deriv         <- Inf
+   while((iter < max.iter) & (abs(deriv) > stop.deriv)) {
+     iter  <- iter + 1
+     sse.1 <- sum((gmp$pcgmp - 6611*gmp$pop^beta)^2)
+     sse.2 <- sum((gmp$pcgmp
+                   - 6611*gmp$pop^(beta + deriv.step))^2)
+     deriv <- (sse.2 - sse.1)/deriv.step
+     beta  <- beta - step.scale*deriv
+   }
+   fit <- list(beta = beta, iteration = iter,
+               converged = (iter < max.iter))
+   return(fit)
+ }
```

Second Fix

Problem: Have to rerun if we want to change defined parameters.
Solution: Let's make them arguments (with default values) of the function.

Second Fix

```
> est.scaling.exponent <- function(beta, beta_0 = 6611,
+   max.iter = 100, stop.deriv = .01, deriv.step = .001,
+   step.scale = 1e-15) {
+
+   iter  <- 0
+   deriv <- Inf
+
+   while((iter < max.iter) & (abs(deriv) > stop.deriv)) {
+     iter  <- iter + 1
+     sse.1 <- sum((gmp$pcgmp - beta_0*gmp$pop^beta)^2)
+     sse.2 <- sum((gmp$pcgmp
+                   - beta_0*gmp$pop^(beta + deriv.step))^2)
+     deriv <- (sse.2 - sse.1)/deriv.step
+     beta  <- beta - step.scale*deriv
+   }
+   fit <- list(beta = beta, iteration = iter,
+               converged = (iter < max.iter))
+   return(fit)
+ }
```

Third Fix

Problem: Don't need to write out the SSE calculations twice in the body of the function.

Solution: Write a `SSE()` function.

Third Fix

```
> est.scaling.exponent <- function(beta, beta_0 = 6611,
+   max.iter = 100, stop.deriv = .01, deriv.step = .001,
+   step.scale =1e-15) {
+
+   iter  <- 0
+   deriv <- Inf
+
+   sse <- function(b) {sum((gmp$pcgmp - beta_0*gmp$pop^b)^2)}
+
+   while((iter < max.iter) & (abs(deriv) > stop.deriv)) {
+     iter  <- iter + 1
+     deriv <- (sse(beta + deriv.step) - sse(beta))/deriv.step
+     beta  <- beta - step.scale*deriv
+   }
+   fit <- list(beta = beta, iteration = iter,
+               converged = (iter < max.iter))
+   return(fit)
+ }
```

`sse()` is declared inside the function so it's not added to the global environment.

Fourth Fix

Problem: Locked into using specific columns of `gmp`: if we want to use a different data set, have to rewrite the function.

Solution: Make them arguments.

Fourth Fix

```
> est.scaling.exponent <- function(beta, beta_0 = 6611,
+   response = gmp$pcgmp, predictor = gmp$pop,
+   max.iter = 100, stop.deriv = .01, deriv.step = .001,
+   step.scale =1e-15) {
+
+   iter  <- 0
+   deriv <- Inf
+
+   sse <- function(b) {sum((response - beta_0*predictor^b)^2)}
+
+   while((iter < max.iter) & (abs(deriv) > stop.deriv)){
+     iter  <- iter + 1
+     deriv <- (sse(beta + deriv.step) - sse(beta))/deriv.step
+     beta  <- beta - step.scale*deriv
+   }
+   fit <- list(beta = beta, iteration = iter,
+               converged = (iter < max.iter))
+   return(fit)
+ }
```

Fifth Fix

Problem: Want to make it easy for humans to read.
Solution: Change the `while` loop to `for` loop with a `break()` command.

Fifth Fix

```
> est.scaling.exponent <- function(beta, beta_0 = 6611,
+   response = gmp$pcgmp, predictor = gmp$pop,
+   max.iter = 100, stop.deriv = .01, deriv.step = .001,
+   step.scale =1e-15) {
+
+   iter <- 0
+   deriv <- Inf
+
+   sse <- function(b) {sum((response - beta_0*predictor^b)^2)}
+
+   for (i in 1:max.iter) {
+         iter  <- iter + 1
+     deriv <- (sse(beta + deriv.step) - sse(beta))/deriv.step
+     beta  <- beta - step.scale*deriv
+     if (abs(deriv) < stop.deriv) {break()}
+   }
+   fit <- list(beta = beta, iteration = iter,
+                converged = (iter < max.iter))
+   return(fit)
+ }
```

Summary

Final code is shorter, more flexible, easier to understand, and more re-usable!

- *Exercise*: Run the code with the default values to get an estimate of β. Plot the curve with the data points to check out the fit.
- *Exercise*: Randomly remove one data point – how much does the estimate change?
- *Exercise*: Run the code from different starting points – how much does the estimate change?

Assessing Model Accuracy

Selecting a Model

Let's recall the grocery store example from Lecture 2 on multiple linear regression. How do we know if the model we selected is a good fit?

Selecting a Model

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Example

A large national grocery retailer tracks productivity and costs of its facilities closely. Consider a data set obtained from a single distribution center for a one-year period. Each data point for each variable represents one week of activity. The variables included are number of cases shipped in thousands (X_1), the indirect costs of labor as a percentage of total costs (X_2), a qualitative predictor called holiday that is coded 1 if the week has a holiday and 0 otherwise (X_3), and total labor hours (Y).

The Model

Example

```
> Grocery <- read.table("Kutner_6_9.txt", header=T)
> lm0     <- lm(Y ~ X1 + X2 + X3, data = Grocery)
> lm0
```

```
Call:
lm(formula = Y ~ X1 + X2 + X3, data = Grocery)

Coefficients:
(Intercept)           X1           X2           X3
  4149.8872       0.7871     -13.1660     623.5545
```

$$\begin{aligned}\widehat{\text{LaborHours}} &= 4149.89 + 0.79 \times \text{ NumCases} \\ &\quad - 13.17 \times \text{ IndirectCosts } + 623.55 \times \text{ Holiday}\end{aligned}$$

Selecting a Model

Some Questions

- The coefficient for number of cases was nearly 0, should this be included as a predictor in the model?
- Suppose we have additional information like weather data, should it be included in the model?
- Is linear regression the best predictive model to use with this data?

Selecting a Model

Some Questions

- The coefficient for number of cases was nearly 0, should this be included as a predictor in the model?
- Suppose we have additional information like weather data, should it be included in the model?
- Is linear regression the best predictive model to use with this data?

Often we must compare multiple models. How do we know which is best?

Quality of Fit

To evaluate the performance of a method on a given data set, we need to measure how well its predictions match the observed data.

- Linear regression uses **mean squared error** (MSE):

$$\frac{1}{n}\sum_{i=1}^{n}(Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_{i1} - \ldots - \hat{\beta}_p X_{ip})^2.$$

Called the **training MSE** since it's calculated on the training data.

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  Called the **training MSE** since it's calculated on the training data.

- But what we actually want to minimize is the **test MSE**:

$$Ave(Y_{test} - \hat{\beta}_0 - \hat{\beta}_1 X_{test,1} - \ldots - \hat{\beta}_p X_{test,p})^2,$$

  using **test** data that was not used to fit the model.

We are interested in the accuracy of the predictions that we obtain when we apply our method to previously unseen **test data**.

The Test MSE

How do we minimize the test MSE?

- Sometimes have a **test** dataset (that wasn't used to train the model.)

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The Test MSE

How do we minimize the test MSE?

- Sometimes have a **test** dataset (that wasn't used to train the model.)
- What if no **test** data is available?
- Idea: Use the model with the lowest **training** MSE.
    - Unfortunately, no guarantee that the method with the lowest **training** MSE will also have the lowest **test** MSE.
- This week we'll learn a strategy for estimating the **test** MSE when no **test** data is available: *Cross-validation*.

Section IV

Classification

What is Classification?

- We studied linear regression for use when we want to predict a quantitative response variable.
- What if we have a categorical response variable?
- The study of predicting categorical response variables is called **classification**.

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- What if we have a categorical response variable?
- The study of predicting categorical response variables is called **classification**.

Examples

- A person has symptoms that could possibly be attributed to one of three medical conditions. Which condition does he have?
- A bank must be able to determine whether an online transaction is fraudulent, on the basis of the user's IP address, past transaction history, etc.
- Using DNA sequence data for patients with and without a disease, a biologist would like to figure out which DNA mutations cause diseases and which do not.

Types of Classifiers

Many methods of classification:

- Logistic Regression.
- Linear Discriminant Analysis.
- K Nearest Neighbors.
- Trees and Random Forests.
- Support Vector Machines

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Set-up

- Just as in regression, we have a set of training observations (data):

$$(X1, Y1), (X2, Y2), \ldots, (Xn, Yn), \quad Y1, Y2, \ldots, Yn \text{ categorical.}$$

- Use the data to build the classifier.
- We want our classifier to perform well not only on the training data, but also on test observations that were not used to build the classifier.

Assessing the Accuracy

Recall, for linear regression we calculated to **training** mean squared error:

$$\frac{1}{n}\sum_{i=1}^{n}(Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_{i1} - \ldots - \hat{\beta}_p X_{ip})^2$$

Assessing the Accuracy

Recall, for linear regression we calculated to **training** mean squared error:

$$\frac{1}{n}\sum_{i=1}^{n}(Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_{i1} - \ldots - \hat{\beta}_p X_{ip})^2$$

For classification, we study the **error rate**:

$$\frac{1}{n}\sum_{i=1}^{n}\mathbb{I}[Y_i \neq \hat{Y}_i].$$

- $\hat{Y}_i$ is the predicted classification for the i^{th} observation.
- $\mathbb{I}[Y_i \neq \hat{Y}_i]$ is an *indicator variable* that equals 1 if $Y_i \neq \hat{Y}_i$ and 0 if $Y_i = \hat{Y}_i$.
- If $\mathbb{I}[Y_i \neq \hat{Y}_i] = 0$ then the i^{th} observation was classified correctly.
- The *error rate* computed the fraction of incorrect classifications.

Assessing the Accuracy

- Similarly to the regression case, the following is referred to as the **training** error rate:
$$\frac{1}{n}\sum_{i=1}^{n}\mathbb{I}[Y_i \neq \hat{Y}_i].$$
- The **test** error rate associated with a set of **test** observations (X_{test}, Y_{test}) is given by
$$Ave(\mathbb{I}[Y_{test} \neq \hat{Y}_{test}]).$$
- A good classifier is one for which the **test** error rate is the smallest.

Bayes Classifier

The best classifier (in terms of **test** error) *assigns each observation to the most likely class*, given its predictor values.

Bayes Classifier

The best classifier (in terms of **test** error) *assigns each observation to the most likely class*, given its predictor values.

- Assign test observation with predictor vector X_{test} to the class j for which

$$Pr(Y = j | X = X_{test})$$

  is largest.
- This is a *conditional probability*. Recall 'Bayes Rule':

$$Pr(A|B) = \frac{Pr(A \text{ and } B)}{Pr(B)}$$

Bayes Classifier

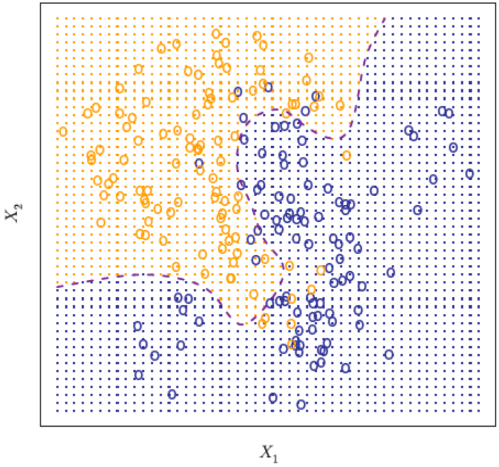
Consider a two-class problem, meaning Y_{test} is either class A or class B.

The Bayes classifier predicts:

$$\begin{cases} \text{Class A} & \text{if } Pr(Y = A | X = X_{test}) > 0.5, \\ \text{Class B} & \text{otherwise.} \end{cases} \tag{1}$$

Bayes Classifier Example [1]

Simulated data of 100 observations. Response Y either blue or orange, with two predictors $X1$ and $X2$. The purple line represents the **Bayes decision boundary**.



K Nearest Neighbors

In theory would like to always use the Bayes classifier. In practice, don't know $Pr(Y|X)$!

K Nearest Neighbors (KNN)

- Estimates $Pr(Y|X)$ and then classifies observations to the class with highest estimated probability.

K Nearest Neighbors

In theory would like to always use the Bayes classifier. In practice, don't know $Pr(Y|X)$!

K Nearest Neighbors (KNN)

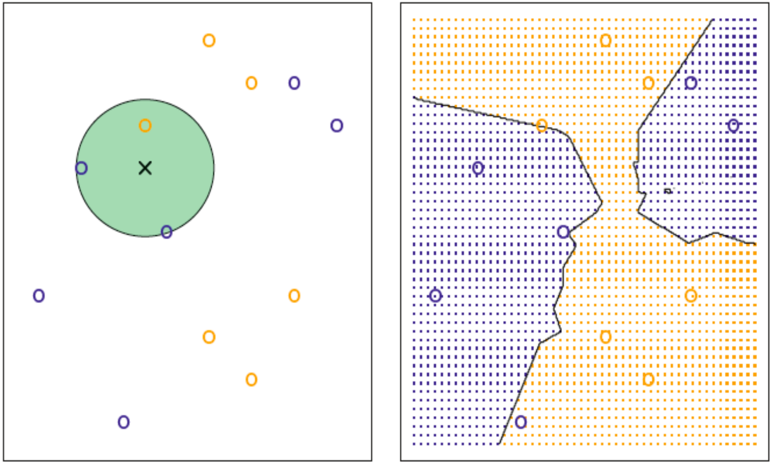
- Estimates $Pr(Y|X)$ and then classifies observations to the class with highest estimated probability.
- Given a positive integer K and a test observation X_{test}:
  - Identify K points in training data closest to X_{test}. Label $\mathcal{N}_{test}$.
  - Estimate conditional probability for class j as fraction of points in $\mathcal{N}_{test}$ whose response values equal j:

$$Pr(Y = j|X = X_{test}) = \frac{1}{K} \sum_{i \in \mathcal{N}_{test}} \mathbb{I}(Y_i = j).$$

  - Classify the test observation to class with the largest probability.

KNN Classifier Example [2]

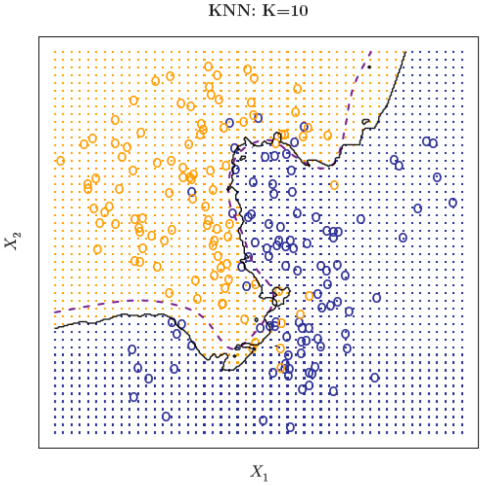
Training data with six blue and six orange observations. Use $K = 3$. **KNN decision boundary** shown in black.



[1]Image from 'Introduction to Statistical Learning'.

KNN Classifier Example [3]

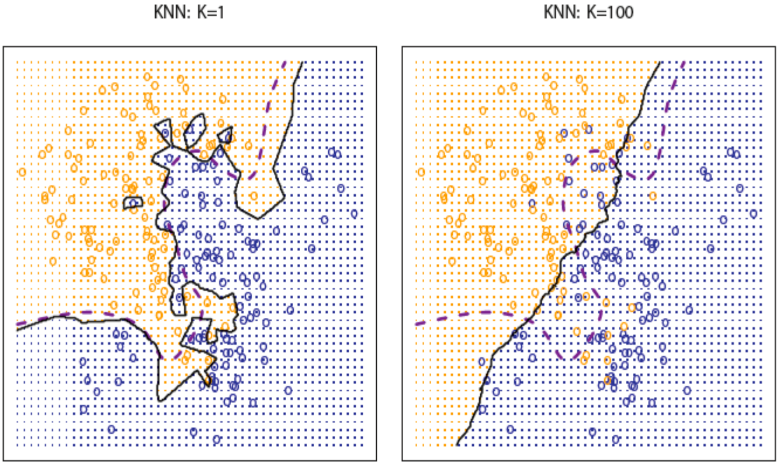
Though simple, KNN can be surprisingly close to Bayes optimal classifier!



[1]Image from 'Introduction to Statistical Learning'.

KNN Classifier Example [4]

Choice of K matters!



[1]Image from 'Introduction to Statistical Learning'.

Assessing Model Accuracy

As with regression, **training** error not a good predictor of **test** error. (Previous example!)

Classification: An Example

Can we predict the direction of the stock market today using the previous two days' movements?

Classification: An Example

Can we predict the direction of the stock market today using the previous two days' movements?

```
> # install.packages("ISLR")
> library(ISLR)
> head(Smarket, 3)
```

```
  Year  Lag1   Lag2   Lag3   Lag4   Lag5 Volume  Today
1 2001 0.381 -0.192 -2.624 -1.055  5.010 1.1913  0.959
2 2001 0.959  0.381 -0.192 -2.624 -1.055 1.2965  1.032
3 2001 1.032  0.959  0.381 -0.192 -2.624 1.4112 -0.623
  Direction
1        Up
2        Up
3      Down
```

Classification: An Example

Variables

- **Year**: The year that the observation was recorded
- **LagX**: Percentage return X days ago.
- **Volume**: Volume of shares traded (number of daily shares traded in billions)
- **Today**: Percentage return for today
- **Direction**: A factor with levels Down and Up indicating whether the market had a positive or negative return on a given day.

Classification: An Example

Variables

- **Year**: The year that the observation was recorded
- **LagX**: Percentage return X days ago.
- **Volume**: Volume of shares traded (number of daily shares traded in billions)
- **Today**: Percentage return for today
- **Direction**: A factor with levels Down and Up indicating whether the market had a positive or negative return on a given day.

```
> mean(Smarket$Lag1[Smarket$Direction == "Up"])
```

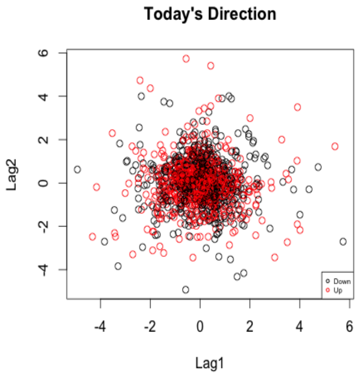
```
[1] -0.03969136
```

```
> mean(Smarket$Lag1[Smarket$Direction == "Down"])
```

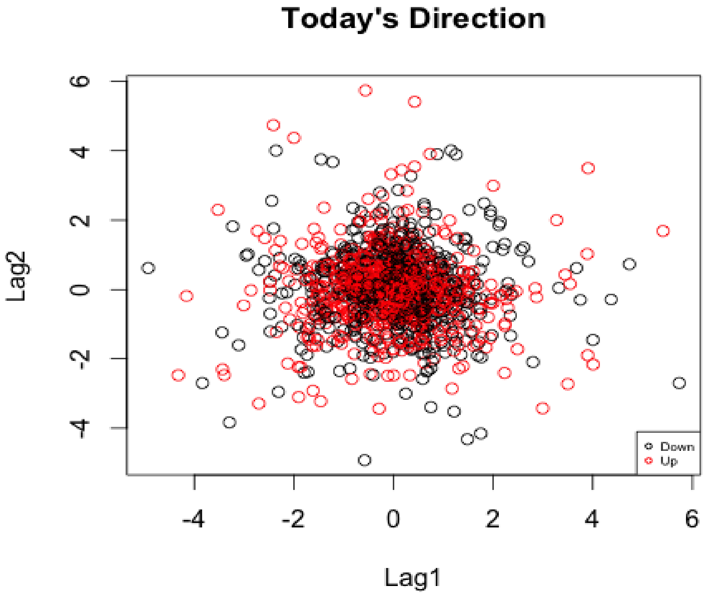
```
[1] 0.05068605
```

Classification: An Example

```
> plot(Smarket$Lag1, Smarket$Lag2, col = Smarket$Direction,
+       xlab="Lag1", ylab="Lag2", main="Today's Direction")
> legend("bottomright", legend = levels(Smarket$Direction),
+         col=1:length(levels(Smarket$Direction)), pch=1)
```



Classification: An Example



Classification: An Example

Procedure

For a new point $(Lag1_{new}, Lag2_{new})$,

- Calculate the Euclidean distance between the new point and all data points. For a data point $(L1, L2)$,

$$\text{dist}^2 = (Lag1_{new} - L1)^2 + (Lag2_{new} - L2)^2.$$

- Create the set $\mathcal{N}_{new}$ containing the K closest points.
- Determine the number of 'UPs' and 'DOWNs' in $\mathcal{N}_{new}$ and classify the new point.

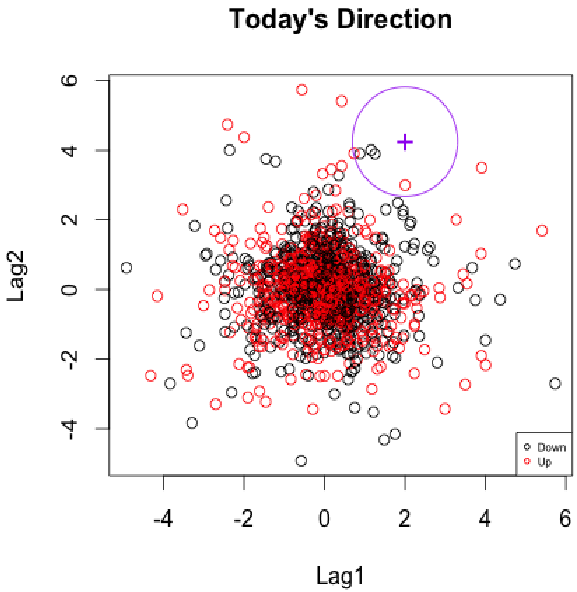
Classification: An Example

Coding The Procedure

```
> K             <- 5
> Lag1.new      <- 2
> Lag2.new      <- 4.25
> # K = 5 and new point (2, 4.25).
>
> dists         <- sqrt((Smarket$Lag1 - Lag1.new)^2
+                    + (Smarket$Lag2 - Lag2.new)^2)
> neighbors    <- order(dists)[1:K]
> neighb.dir <- Smarket$Direction[neighbors]
> choice       <- names(which.max(table(neighb.dir)))
> choice
```

```
[1] "Down"
```

Classification: An Example



Check Yourself

Task

Write a function called `KNN.decision` that returns the class decision for any new point $(Lag1_{new}, Lag2_{new})$ and any choice of K (with $K = 5$) as default.

Check Yourself

One Solution:

```
> KNN.decision <- function(Lag1.new, Lag2.new, K = 5,
+                          Lag1 = Smarket$Lag1,
+                          Lag2 = Smarket$Lag2,
+                          Dir = Smarket$Direction) {
+   n <- length(Lag1)
+   stopifnot(length(Lag2) == n, length(Lag1.new) == 1,
+             length(Lag2.new) == 1, K <= n)
+
+   dists <- sqrt((Lag1-Lag1.new)^2 + (Lag2-Lag2.new)^2)
+
+   neighbors  <- order(dists)[1:K]
+   neighb.dir <- Dir[neighbors]
+   choice     <- names(which.max(table(neighb.dir)))
+   return(choice)
+ }
```

Testing Our Model

Let's build our model using data from 2001 - 2004 and use the 2005 data as a test. Can we predict market direction better than a random guess?

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Let's build our model using data from 2001 - 2004 and use the 2005 data as a test. Can we predict market direction better than a random guess?

```
> test  <- Smarket[Smarket$Year == 2005, ]
> train <- Smarket[Smarket$Year != 2005, ]
> n.test <- nrow(test)
> predictions <- rep(NA, n.test)
> for (i in 1:n.test){
+   predictions[i] <- KNN.decision(test$Lag1[i],test$Lag2[i],
+                      Lag1 = train$Lag1,Lag2 = train$Lag2,
+                      Dir = train$Direction)
+ }
> test.error <- sum(predictions != test$Direction)/n.test
> test.error
```

```
[1] 0.515873
```

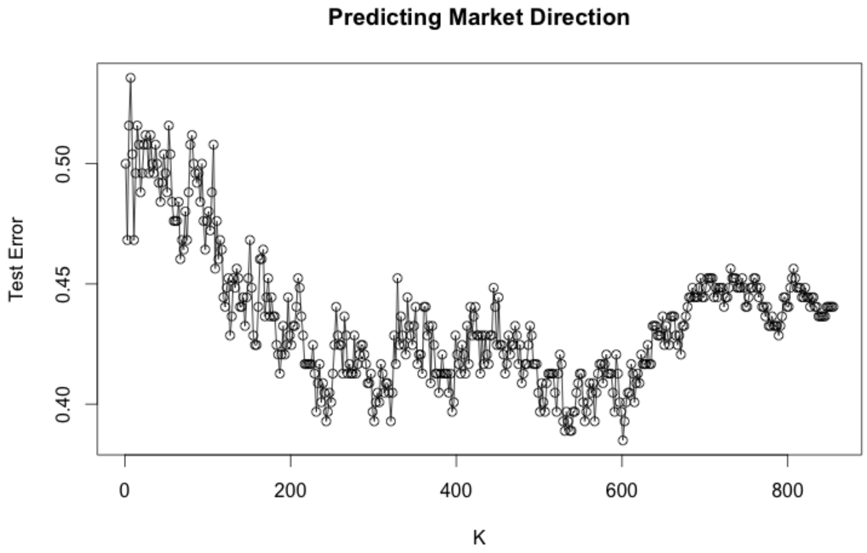
Testing Our Model: Another Try

Let's build our model using data from 2001 - 2004 and use the 2005 data as a test. Can we predict market direction better than a random guess?

```
> test  <- Smarket[Smarket$Year == 2005, ]
> train <- Smarket[Smarket$Year != 2005, ]
> n.test <- nrow(test)
> predictions <- rep(NA, n.test)
> for (i in 1:n.test){
+   predictions[i] <- KNN.decision(test$Lag1[i],test$Lag2[i],
+                                  K = 7,
+                                  Lag1 = train$Lag1,Lag2 = train$Lag2,
+                                  Dir = train$Direction)
+ }
> test.error <- sum(predictions != test$Direction)/n.test
> test.error
```

```
[1] 0.5357143
```

Classification: An Example



Optional Reading

- Chapter 4 (Classification) and Chapter 5 (Cross-Validation) in An Introduction to Statistical Learning.
- Chapter 10 (Writing Your Own Functions) in An Introduction to `R`